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LARGE EDDY SIMULATION OF TURBULENCE: A SUBGRID SCALE MODEL INCLUDING SHEAR, VORTICITY, ROTATION, AND BUOYANCY

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ABSTRACT

The Reynolds numbers that characterize geophysical and astrophysical turbulence (Re $\approx 10^8$ for the planetary boundary layer and Re $\approx 10^{14}$ for the Sun's interior) are too large to allow a direct numerical simulation (DNS) of the fundamental Navier-Stokes and temperature equations. In fact, the spatial number of grid points $N \sim \mathrm{Re}^{9/4}$ exceeds the computational capability of today's supercomputers.

Alternative treatments are the *ensemble-time average* approach, and/or the *volume average* approach. Since the first method (Reynolds stress approach) is largely analytical, the resulting turbulence equations entail manageable computational requirements and can thus be linked to a stellar evolutionary code or, in the geophysical case, to general circulation models. In the volume average approach, one carries out a large eddy simulation (LES) which resolves *numerically* the largest scales, while the unresolved scales must be treated *theoretically* with a subgrid scale model (SGS). Contrary to the ensemble average approach, the LES+SGS approach has considerable computational requirements. Even if this prevents (for the time being) a LES+SGS model to be linked to stellar or geophysical codes, it is still of the greatest relevance as an "experimental tool" to be used, inter alia, to improve the parameterizations needed in the ensemble average approach. Such a methodology has been successfully adopted in studies of the convective planetary boundary layer.

Experience with the LES+SGS approach from different fields has shown that its reliability depends on the healthiness of the SGS model for numerical stability as well as for physical completeness. At present, the most widely used SGS model, the Smagorinsky model, accounts for the effect of the shear induced by the large resolved scales on the unresolved scales but does not account for the effects of buoyancy, anisotropy, rotation, and stable stratification. The latter phenomenon, which affects both geophysical and astrophysical turbulence (e.g., oceanic structure and convective overshooting in stars), has been singularly difficult to account for in turbulence modeling. For example, the widely used model of Deardorff has not been confirmed by recent LES results. As of today, there is no SGS model capable of incorporating *buoyancy, rotation, shear, anisotropy, and stable stratification (gravity waves)*.

In this paper, we construct such a model which we call CM (complete model). We also present a hierarchy of simpler algebraic models (called AM) of varying complexity. Finally, we present a set of models which are simplified even further (called SM), the simplest of which is the Smagorinsky-Lilly model. The incorporation of these models into the presently available LES codes should begin with the SM, to be followed by the AM and finally by the CM.

Subject headings: convection — methods: analytical — methods: numerical — turbulence

A numerical procedure without a turbulence model stands in the same relation to a complete calculation as an ox does to a bull—PETER BRADSHAW

1. INTRODUCTION

Turbulence is not a property of a fluid but a property of a fluid in motion. Thus, its maintenance requires continuous nourishment, a source of external energy which, fed at the largest scales, is transferred to all other scales by the nonlinear interactions. The latter, by definition, conserve energy and so the power ϵ fed into the system at the largest scales is found unaltered at the dissipation scale l_d where molecular processes dissipate it into heat. It must be stressed that the amount of energy dissipated is *not* determined by the small scales; the latter determine only the scales at which dissipation occurs. Thus, l_d depends on only two quantities: the input power ϵ (ergs g^{-1} s^{-1}) that characterizes the source, and kinematic viscosity ν (cm^2 s^{-1}) that characterizes the sink. From dimensional arguments it follows that

$$l_d = (\nu^3\epsilon^{-1})^{1/4} . \quad (1)$$

Since ϵ is determined by the largest scales which have characteristic velocities U and length scales L, one of the most basic relations in turbulence theory dictates that (Batchelor 1971)

$$\epsilon = U^3/L . \quad (2)$$

Insertion of equation (2) into equation (1) yields the ratio of the largest scales L to the dissipation scale l_d

$$\frac{L}{l_d} = \mathrm{Re}^{3/4}, \quad \mathrm{Re} = \frac{UL}{\nu} , \quad (3)$$

where Re is the Reynolds number. The large values of L and the small values of ν that characterize geophysical (Wyngaard 1992) and astrophysical settings (Spruit, Nordlund, & Title 1990) militate to create huge Reynolds numbers, $Re \approx 10^8$ for the Earth's boundary layer and $Re \approx 10^{14}$ for the Sun's turbulent convection. By contrast, in many laboratory and engineering turbulent flows, $Re \approx 10^4$. Herring (1987) has also pointed out that for a fixed Rayleigh number, the Reynolds number R_λ ($=u\lambda\nu^{-1}$, where λ is the Taylor microscale λ and u is the rms turbulent velocity) decreases with the Prandtl number as $\sigma^{-5/9}$; in the Sun, $\sigma \sim 10^{-10}$ (Massaguer 1990). Since turbulence is three-dimensional, the number of spatial grid points N_s thus grows as

$$N_s \sim Re^{9/4} . \tag{4}$$

If we employ R_λ, we have

$$N_s \sim R_\lambda^{36/7} . \tag{5}$$

In the case of solar convection, a full three-dimensional simulation would require $\sim 10^{30}$ grid points, while in the case of the planetary boundary layer one would need 10^{18} grid points. These numbers must be contrasted with today's supercomputers that can handle at most 10^9 grid points.

These relations highlight what is perhaps the most distinguishing feature of turbulence, the richness of the dynamical scales involved. How to describe all the strongly and nonlinearly interacting scales has been the major goal of turbulence modeling.

The plan of the paper is as follows: in § 2 we discuss the general spirit and limitations behind large eddy simulation (LES), direct numerical simulation (DNS), and ensemble average techniques. In § 3 we discuss the problem of deriving the Reynolds stresses and convective fluxes and cite some well-known models. In § 4 we discuss the specific case of turbulent convection in stellar cases, and we present a series of physical arguments that argue against the use of the simple "turbulent viscosity" approximation for the Reynolds stresses. In § 5 we present the *complete model* (CM): a set of differential equations that govern the Reynolds stresses, the convective flux, the temperature variance as well as the dissipation rates of turbulent kinetic energy and temperature variance. In § 6 we present the *algebraic models* (AMs): a class of algebraic Reynolds stress models which constitute a considerable simplification of the AM since the two primary quantities, the Reynolds stresses and the convective fluxes, are given in algebraic form. We present four AMs of decreasing complexity, the last model being entirely algebraic. In order to quantify the effects of several of the physical ingredients of the models, in § 7 we present a set of *Simplified Models* (SMs), the simplest of which is the Smagorinsky-Lilly model. In § 8 we present some general conclusions. In Appendices A–C, we present a detailed derivation of the CM. In Appendix D we present a new formulation for the third-order moments to be used in subgrid scale (SGS) modeling. In Appendix E we present the numerical values of the constants entering the models.

2. DNS, LES, AND ENSEMBLE AVERAGE

2.1. *Direct Numerical Simulations*

This approach, which has met with considerable success in engineering problems, consists of solving the basic Navier-Stokes and energy equations using a Direct Numerical Simulation (DNS) technique whereby one resolves numerically all the dynamical scales from L to the dissipation length scale l_d. Because of equation (4), the DNS method is limited to low values of Re (Corrsin 1951; Rogallo 1981; Rogallo & Moin 1984; Reynolds 1990).

2.2. *Ensemble–Time Average*

This method was proposed last century by O. Reynolds. The Navier-Stokes equations of motion are first averaged over a infinite ensemble of realizations so as to obtain the equations for the ensemble mean fields. If one considers time averages, the time considered must be larger than the timescale of turbulence but smaller than the timescale of the mean motion (Rodi 1984). If v_i represents the total velocity field, U_i the mean field, and u_i the fluctuating part, $v_i = U_i + u_i$, with $\bar{u}_i = 0$, the averaging process leads to the following equation for U_i:

$$\frac{\partial}{\partial t} U_i + U_j \frac{\partial}{\partial x_j} U_i = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\nu \frac{\partial U_i}{\partial x_j} - \overline{u_i u_j}\right) . \tag{6}$$

An analogous calculation gives the equation for the mean temperature T (χ is the thermometric conductivity)

$$\frac{\partial T}{\partial t} + U_i \frac{\partial T}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\chi \frac{\partial T}{\partial x_i} - \overline{u_i \theta}\right) . \tag{7}$$

Equations (6) and (7) for the mean variables U_i and T look like the original equations describing the laminar flow: turbulence enters through the nonlinear interactions that give rise to the new functions

$$\overline{u_i u_j} \quad \text{and} \quad \overline{u_i \theta} \tag{8}$$

which are called *Reynolds stresses and turbulent heat fluxes*. Until one devises a model for these new functions, equations (6)–(7) are "not closed" and thus cannot be solved.

2.3. *Large Eddy Simulations*

The scales of a highly turbulent flow can be separated into two broad categories with quite different characteristics: *large eddies* contain most of the energy, do most of the transporting, are diffusive, anisotropic, long-lived, inhomogeneous, ordered, and dependent on the boundaries and thus difficult to model analytically. On the other hand, *small eddies* are dissipative, isotropic, short-lived, homogeneous, random, and universal, and thus more amenable to theoretical modeling (Schumann, 1991). The conceptual basis of the LES approach is therefore that the largest scales, in view of their complexity, should not be modeled theoretically, but rather explicitly numerically simulated, while the smaller scales that cannot be numerically resolved should be modeled via a SGS model, for which one can use any of the Reynolds stress models discussed in this paper (for the foundations of the LES method, see Voke & Collins 1983; Markatos 1987; Yoshizawa 1987; Grotzbach 1987; Reynolds 1990; for a spectral LES, see Metais & Lesieur 1992).

Historically, the LES method was first applied by Deardorff (1970) to study plane channel flow using the SGS model of Smagorinsky (1963) which we shall discuss below. Moin & Kim (1982) reexamined channel flow; Grotzbach & Schumann (1979) studied temperature fluctuations and heat transfer in channel flows; Biringen & Reynolds (1981) studied free-shear turbulent boundary layer while Antonopolous-Domis (1981a, b) used LES to study the characteristics of a passive scalar in homogeneous turbulence.

The widest application of LES (second only to engineering) has occurred in geophysics, specifically in the treatment of the strongly *convective boundary layer* through the work of Wyngaard (1984), Moeng (1984, 1986), Moeng & Wyngaard (1989), Mason & Thomson (1987), Mason (1989), Mason & Derbyshire (1990), Mason & Thomson (1992), Nieuwstadt & de Valk (1987), Schmidt & Schumann (1989), Sykes & Henn (1989), Nieuwstadt (1991), and Mason (1994). The results of the four major LES codes have recently been compared and found to be in excellent agreement (Nieuwstadt et al. 1991). For an update of LES techniques applied to engineering, laboratory, and geophysical flows, see Galperin (1992). Some of the main properties of the strongly convective planetary boundary layer (PBL) may be of interest (Zeman 1981; Wyngaard 1992): extent of the convective layer, $d \sim 1$ km; pressure scale height $H_p \sim 7$ km; Reynolds number $Re \sim 10^8$; Taylor microscale $\lambda \sim 10^{-4}d$ ($\lambda^2 = \nu v^2/\epsilon$), which marks roughly the small-scale end of the Kolmogorov spectrum; length scale l and velocity v of the flux carrying eddies $l \sim d$, $v \sim 1$ m s^{-1}; dissipation scale $l_d \sim \lambda(\epsilon\nu)^{1/4}v^{-1} \sim 10^{-6}d$, dissipation rate of kinetic energy $\epsilon \sim v^3/l \sim 10$ cm^2 s^{-3}.

It may be of interest to remark that in the stellar case not only is the value of Re several orders of magnitude larger ($\sim 10^{14}$), but the ratio d/H_p is of $O(1)$, while in the PBL is $O(10^{-1})$. Thus, in principle, the thin-layer approximation is satisfied in the PBL but not in stellar interiors, as discussed in some detail in Canuto (1993, hereafter Paper II), where such an approximation was avoided.

Mathematically, a LES procedure begins with the introduction of a volume average through a filter operation whereby all scales larger than a given size Δ are fully resolved while all the scales smaller than Δ have to be modeled. Consider the Navier-Stokes equations for an inviscid, incompressible fluid of total velocity field v_i,

$$\frac{\partial}{\partial t} v_i + \frac{\partial}{\partial x_j} v_i v_j = -\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2}{\partial x_j^2} v_i , \quad \frac{\partial}{\partial x_j} v_j = 0 . \qquad (9)$$

The process of filtering all scales smaller than a given size Δ is accomplished via a filter operation whereby given a variable $f(x)$, one defines a filtered $\bar{f}$ through

$$\bar{f}(x) = \int G_\Delta(x \mid x') f(x') dx' , \qquad (10)$$

where $G_\Delta(x \mid x')$ is the filter function with a characteristic length scale Δ. Several filters have been proposed in the literature: Gaussian, box, sharp, etc. For a specific form of the filter function, see equation (6) of Marcus (1986). Applying equation (10) to equation (9), one obtains

$$\frac{\partial}{\partial t} \bar{v}_i + \frac{\partial}{\partial x_j} \overline{v_i v_j} = -\frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial^2}{\partial x_j^2} \bar{v}_i . \qquad (11a)$$

As Ferziger (1976) has remarked, one is now faced with the "archetypical problem of turbulence," the need to specify an average of a product, $\overline{v_i v_j}$. As a first step one rewrites equation (11a) in the form

$$\frac{\partial}{\partial t} \bar{v}_i + \frac{\partial}{\partial x_j} \bar{v}_i \bar{v}_j = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \tau_{ij} , \qquad (11b)$$

where

$$\tau_{ij} = \bar{v}_i \bar{v}_j - \overline{v_i v_j} . \qquad (11c)$$

In this way, the form of equation (11b) is the same as the original equation (9), except that the viscous stress is now replaced by the stress τ_{ij}. It is instructive to analyze τ_{ij} in more detail. In analogy with the Reynolds method discussed above, one writes

$$v_i = \bar{v}_i + u_i , \qquad (12)$$

where a bar indicates the filtered, fully resolved large-scale velocity field, and u_i represents the subgrid, unresolved velocity field. Thus,

$$-\tau_{ij} = \overline{\bar{v}_i \bar{v}_j} - \bar{v}_i \bar{v}_j + \overline{u_i \bar{v}_j} + \overline{u_j \bar{v}_i} + \overline{u_i u_j} , \qquad (13)$$

where the first two terms are called the Leonard terms. Leonard (1974) proposed that since the filtered velocity is a fairly smooth function, one can use a Taylor expansion to obtain

$$\overline{\bar{v}_i \bar{v}_j} = \bar{v}_i \bar{v}_j + \frac{\Delta^2}{24} \frac{\partial^2}{\partial x_k^2} \bar{v}_i \bar{v}_j . \qquad (14a)$$

Analogously, Clark, Ferziger, & Reynolds (1976) suggested the expression

$$\overline{u_i \bar{v}_j} = -\frac{\Delta^2}{24} \bar{v}_j \frac{\partial^2}{\partial x_k^2} \bar{v}_i , \qquad (14b)$$

so that finally

$$-\tau_{ij} = \overline{u_i u_j} + \frac{\Delta^2}{12} \left(\frac{\partial \bar{v}_i}{\partial x_k}\right)\left(\frac{\partial \bar{v}_j}{\partial x_k}\right) . \qquad (14c)$$

On the other hand, Bardina, Ferziger, & Reynolds (1980) suggested to approximate the cross-terms, third and fourth terms in equation (13), as follows:

$$\overline{u_i \bar{v}_j} + \overline{u_j \bar{v}_i} = \bar{v}_i \bar{v}_j - \bar{\bar{v}}_i \bar{\bar{v}}_j , \qquad (15a)$$

so that

$$-\tau_{ij} = \overline{u_i u_j} + \overline{\bar{v}_i \bar{v}_j} - \bar{\bar{v}}_i \bar{\bar{v}}_j . \qquad (15b)$$

In both equation (14c) and equation (15b), the terms involving $\bar{v}$ are known, while the first term must be modeled.

3. REYNOLDS STRESSES

The first proposal to model equation (8) dates back to Boussinesq (1877), who suggested that, in analogy with the viscous stresses, the turbulent stresses be taken proportional to the mean-velocity gradient, the constant of proportionality being interpreted as an *eddy or turbulent viscosity*, ν_t. Specifically, the traceless Reynolds stress

$$b_{ij} = \overline{u_i u_j} - \tfrac{2}{3}\delta_{ij} e \qquad (16a)$$

is modeled as follows:

$$b_{ij} = -2\nu_t S_{ij} , \qquad (16b)$$

where

$$2S_{ij} = \frac{\partial}{\partial x_j} U_i + \frac{\partial}{\partial x_i} U_j . \qquad (16c)$$

Here e is the turbulent kinetic energy $\frac{1}{2}\overline{u_i u_i}$ and S_{ij} is the shear of the mean and/or resolved scales. Substituting equation (16b) into equation (6), we note that the presence of turbulence renormalizes the kinematic viscosity, $\nu \rightarrow \nu + \nu_t$. *The problem now is how to determine* ν_t. The kinetic energy e in eq. (16a) can be absorbed into the pressure gradient term in eq. (6). While the renormalization of ν is an appealing concept, it must be stressed that contrary to the viscous case, where the kinematic viscosity ν is a property of the fluid (irrespectively of its state of motion), the turbulent viscosity ν_t is a property of the fluid in motion and thus in principle unknown until the full dynamical problem is solved. In addition, ν_t can hardly be considered a constant. The shortcomings of equation (16a), when applied to the Sun, will be discussed in § 4 below.

Pursuing the analogy with nonturbulent flows, since the kinematic viscosity is the product of an average velocity times a mean free path, Prandtl (1925) was the first to suggest the concept of "*mixing length*" whereby

$$\nu_t \sim vl \,, \tag{16d}$$

where v is an rms turbulent velocity and l is a mixing length.

3.1. *Zero-Equation Models*

The first model for v is also due to Prandtl (1925) who suggested that

$$v = lS \,, \tag{16e}$$

where $S = (2S_{ij}S_{ij})^{1/2}$ is the mean shear. Thus

$$\nu_t = l^2 S \,. \tag{16f}$$

Equation (16f) is the Prandtl mixing-length model. Equations (16a)–(16f) have become understandably very popular not only because of their simplicity (they are categorized as zero-equation models for there are no dynamical equations to be solved) but also because of their successful application to several types of flows (Schlichting 1969; Rodi 1984). However, the specification of the mixing length remains a major problem especially for flows that deviate from the shear layer types for which the model was originally devised.

3.2. *One-Equation Models*

An improvement over the above description can be achieved if one considers that since the bulk of the kinetic energy of a turbulent flow is concentrated in the largest scales, a physically meaningful scale can be taken to be proportional to $e^{1/2}$. Thus, a more complete parameterization of ν_t can be devised whereby one writes

$$\nu_t = c_\nu e^{1/2} l \,. \tag{17a}$$

This is the Kolmogorov (1942)–Prandtl (1945) formula. Clearly, one must now solve a dynamic equation for e (hence the name, one-equation model). Such an equation is derived in Appendix A (eq. [A26]). For the simpler case in which there are no buoyancy forces, and using equation (16b), the resulting equation is

$$\frac{\partial e}{\partial t} + U_i \frac{\partial e}{\partial x_i} + D_f(e) = \nu_t S^2 - \epsilon \,. \tag{17b}$$

The diffusion term D_f is represented by a third-order moment which must be modeled. For many years, it has been customary to adopt the down-gradient or diffusion approximation discussed in Canuto (1992, hereafter Paper I), § 5. Since, however, this term is not relevant to the present discussion, we shall not discuss it any further. The physical interpretation of equation (17b) is that the time variation of the turbulent kinetic energy is governed by advection and diffusion (the last two terms on the left-hand side), while the first term on the right-hand side represents the source of turbulent energy, specifically, the energy extracted from the mean flow by the interaction between the Reynolds stresses and the shear. The last term in equation (17b) represents the dissipation (sink) of that energy and it occurs at the scales l_d, as discussed previously.

To solve equation (17b), one needs to model ϵ (Appendix C). Since ϵ represents the rate of dissipation of turbulent kinetic energy, we write

$$\epsilon \sim e\tau_\epsilon^{-1} \,. \tag{17c}$$

Since

$$\tau_\epsilon \sim l_\epsilon e^{-1/2} \,, \tag{17d}$$

one has (Batchelor 1971)

$$\epsilon \sim \frac{e^{3/2}}{l_\epsilon} \,. \tag{17e}$$

It has been generally felt that due to the difficulties encountered in defining the dissipation length scale l_ϵ, which in principle need not be the same as the l in equation (17a), the advantages of the one-equation model over the zero-equation model are not overwhelming. The past tendency has been either to work with the zero-equation model or to adopt the two-equation models. The conclusion has recently been challenged by Belcher et al. (1991) who suggest that in the case of inhomogeneous turbulence (e.g., turbulence over a wavy surface) the one-equation model, with a properly prescribed mixing length, is superior to a two-equation model (presumably because in such case, the already heavily parameterized equation for ϵ would require further changes for which one has no guidance).

3.3. *Two-Equation Models*

This approach consists of considering, in addition to the equation for the kinetic energy (17b), an additional equation for the dissipation ϵ, which, because of equation (17e), is equivalent to an equation for the length scale l_ϵ. The resulting model is known as the *K-ϵ model* (kinetic energy-dissipation model, Rodi 1984). The dynamical equation for ϵ can be derived from the basic Navier-Stokes equations (Davidov 1961; Speziale 1991): however, its full form contains a variety of terms that cannot be easily interpreted and are thus difficult to parameterize. A great deal of work over many years has gone into the determination of such an equation, which is discussed in Appendix C. Here, we quote the most common form (we leave out buoyancy and employ the so-called down-gradient or diffusion approximation for the third-order moment $\overline{\epsilon u_i}$; see Papers I and II for a further discussion, as well as Appendix D):

$$\frac{\partial \epsilon}{\partial t} + U_j \frac{\partial \epsilon}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\kappa_t \frac{\partial \epsilon}{\partial x_j}\right) + C_{\epsilon 1}\frac{\epsilon}{e}P - C_{\epsilon 2}\frac{\epsilon^2}{e} \,, \tag{18a}$$

where P stands for the production term

$$P = -b_{ij}S_{ij} = \nu_t S^2 \,. \tag{18b}$$

The model is completed by the addition of the two relations

$$\nu_t = c_\nu \frac{e^2}{\epsilon} \,, \quad \kappa_t = \sigma_t^{-1}\nu_t \,, \tag{18c}$$

where σ_t is the turbulent Prandtl number usually taken to be constant.

It is fair to say that the K-ϵ model, equations (16a), (17b), and (18), has been perhaps the most successful model in dealing with a variety of turbulence problems (Rodi 1984; Speziale 1991; Lang & Shih 1991).

3.4. *The Complete Reynolds Stress Model*

In a way, the K-ϵ model is the best one can do under the assumption that the Reynolds stresses have the form of equation (16a). We have already mentioned that equation (16b) yields incorrect results when applied to the Sun, see equations (21g)–(21h) below. However, historically, Keller & Friedmann (1924) were the first to point out that there is actually no need to postulate equation (16b) since one can derive the exact dynamic equations for the stresses (eq. [8]) directly from the Navier-Stokes equations. Interestingly enough, however, Keller & Friedmann did not derive such equations which appeared only 20 yr later (Chou 1945). Today, the most advanced turbulence models employ this approach which is known as *second-order closure model (SOC)*. The last 40 yr of work in this field have led to considerable progress, and the SOC models have achieved considerable accuracy (Launder, Reece, & Rodi 1975; Lumley 1978; Speziale 1991; Shih & Lumley 1985; Zeman & Lumley 1976, Lumley & Mansfield 1984; Lang & Shih 1991; Papers I and II).

The total number of differential equations governing the turbulent quantities is of course much larger, since

$$\overline{u_i u_j}: \text{six equations}, \quad \overline{u_i \theta}: \text{three equations}\,,$$
$$\overline{\theta^2}: \text{one equation}, \quad \epsilon,\ \epsilon_\theta: \text{two equations}\,. \tag{19}$$

In what follows, we first derive the complete SGS model that includes shear, buoyancy, anisotropy, rotation, and stable stratification. Second, we show that under reasonable assumptions, one can reduce the set of differential equations to a model with only one or two differential equations while the remaining are algebraic relations, thus making the model more tractable. Third, we derive the Boussinesq-Kolmogorov-Prandtl, BKP model (one-equation model), a two-equation model, as well as the Smagorinsky model (zero-equation model).

4. STELLAR TURBULENT CONVECTION

Historically, stellar turbulent convection has been treated using all the three methods described above.

4.1. *Direct Numerical Simulations*

The method has been used by several authors (Cattaneo et al. 1989, 1991; Malagoli, Cattaneo, & Brummel 1990; Toomre et al. 1990) to study convection at relatively low $Re \sim 1200$. As discussed earlier, however, in the case of fully developed solar convection, $Re \sim 10^{14}$.

4.2. *Ensemble–Time Average*

The simplest model corresponds to adopting the analog of equation (16b) for the temperature field,

$$\overline{u_i \theta} = -\chi_t\left[\frac{\partial T}{\partial x_i} - \left(\frac{\partial T}{\partial x_i}\right)_{\rm ad}\right], \tag{20a}$$

where $\chi_t = \nu_t/\sigma_t$ plays the role of a "turbulent conductivity." Using equation (A26) in the stationary limit, with no mean field, $U_i = 0$ and with $D_f = 0$, one obtains

$$\epsilon = \chi_t N^2\,, \tag{20b}$$

where N is the Brunt-Vaisala frequency (α is the volume expansion coefficient):

$$N^2 = -g\alpha\left[\frac{\partial T}{\partial z} - \left(\frac{\partial T}{\partial z}\right)_{\rm ad}\right]. \tag{20c}$$

Next, using equations (17e) and (18c), one obtains

$$e \sim l^2 N^2, \quad \chi_t \sim l^2 N\,, \tag{20d}$$

so that the convective flux, $F_c = c_p \rho \overline{w\theta}$ can be written as

$$F_c \sim (g\alpha)^{1/2} l^2\left[-\frac{\partial T}{\partial z} + \left(\frac{\partial T}{\partial z}\right)_{\rm ad}\right]^{3/2}, \tag{20e}$$

which is the well-known expression provided by the mixing length theory (MLT, Böhm-Vitense 1958). A complete SOC model has been recently developed by Canuto (1992, 1993) and by Xiong (1985, 1986) who has also linked the turbulence model to a stellar structure code (Unno, Kondo, & Xiong 1985; Unno & Kondo 1989).

4.3. *Large Eddy Simulations*

In astrophysical turbulence, the LES techniques have not yet been used as extensively as in geophysics but interesting results are becoming available. Marcus (1986) has discussed the consequences of neglecting the contribution of the SGS as well as that of mimicking them via the "numerical viscosity" that appears in finite difference schemes. He has shown that the latter type of viscosity fails to represent the real turbulent viscosity because it draws energy preferentially from scales of size L rather than from scales of order Δ and thus violates the general principle of an LES, namely a SGS model must leave the largest scales undisturbed while draining energy from scales of order Δ. He has further shown that the "numerical viscosity" actually describes a viscous laminar flow rather than an almost inviscid, turbulent flow, as one need consider (see also Marcus, Press & Teukolsky, 1983).

The following is the simplest SGS model:

$$b_{ij} = -2\nu_t S_{ij}\,, \tag{21a}$$

$$\overline{u_i \theta} = -\chi_t\left[\frac{\partial T}{\partial x_i} - \left(\frac{\partial T}{\partial x_i}\right)_{\rm ad}\right], \tag{21b}$$

$$\chi_t = \nu_t \sigma_t^{-1}\,, \quad \sigma_t = \text{constant}\,. \tag{21c}$$

Neglecting the whole left-hand side of equation (17b),

$$U_i \frac{\partial e}{\partial x_i} \to 0 \quad D_f(e) \to 0\,, \tag{21d}$$

which implies no transport of the small scales by the large scales and no diffusion of the turbulent kinetic energy (a local model for convection), one obtains that production equals dissipation

$$\epsilon = \nu_t S^2\,. \tag{21e}$$

Further employing equation (17e) for ϵ, and equation (17a) for ν_t, one finally obtains assuming $l \sim l_\epsilon \sim \Delta$,

$$\nu_t = (C_s \Delta)^2 S\,, \tag{21f}$$

which is *the Smagorinsky model* (1963) (a complete derivation is given below).

This SGS model has been used by Sofia & Chan (1984), Marcus (1986), Chan & Sofia (1986, 1989), Hossain & Mullan (1991), Fox, Sofia, & Chan (1991), Fox, Theobald, & Sofia (1991), and Xie & Toomre (1991, 1993); these authors treat compressible turbulence but the physical content of their SGS model is the same, see Erlebacher et al. 1992). By contrast, Nordlund (1982), Stein & Nordlund (1989), Stein, Nordlund, & Kuhn (1989), Glatzmaier (1984; 1985a, b; 1987), Gilman & Miller (1986), and Atroshchenko et al. (1989) have used constant eddy viscosity and/or hyperviscosity models (for a recent suggestion how to compute C_s in eq. [21f]; see Germano 1992).

4.4. *Critique of the SGS Model (21)*

The question naturally arises: is the SGS model (eq. [21]) a trustworthy description of turbulence in the presence of convection rather than shear?

a. Model (21) was originally designed to describe shear-generated rather than convection-generated turbulence (which is the case of stellar interiors). An illustration of the shortcoming of the physical content of equation (21a) in dealing with convection in an ensemble average mode comes from considering that in spherical coordinates equation (21a) yields

$$\overline{u_\theta u_\phi} = -\nu_t \frac{\partial \Omega}{\partial \theta} . \quad (21g)$$

In the case of the sun, $\partial\Omega/\partial\theta > 0$ in the northern hemisphere (N) and <0 in southern hemisphere (S). Thus, equation (21g) implies that

$$\overline{u_\theta u_\phi} < 0 \text{ (N)}, \quad \overline{u_\theta u_\phi} > 0 \text{ (S)} , \quad (21h)$$

while observational data indicate the opposite behavior (Rudiger 1989; Pulkkinen et al. 1993).

b. Equation (21a) represents the first term in a Taylor series in the parameter τ/T, where τ is the turbulence timescale and T is the mean flow typical timescale. This can be seen by writing equation (21a) as

$$\frac{b_{ij}}{e} \sim \frac{\nu_t}{Te}(TS_{ij}) \sim \frac{\tau}{T}(TS_{ij}) , \quad (21i)$$

where ν_t is given by equation (18c) and $\tau \sim e/\epsilon \sim l/e^{1/2}$. There is no a priori reason why τ/T be small, especially when one considers that the smallest of the largest scales and the largest of the unresolved (SGS) scales may actually have $\tau \sim T$, giving rise to a *resonance*, which is known to alter the Kolmogorov spectrum (Tchen 1953; Hinze 1975). As recently discussed by Taulbee (1992) and Gatski & Speziale (1993), *nonperturbative* derivations of b_{ij} do in fact exhibit terms of much higher order in (τ/T), up to $(\tau/T)^5$, in Taulbee's case.

c. Equation (21a) requires that the principal axes of the tensors b_{ij} (representing turbulence) and S_{ij} (representing the mean flow) be aligned: this is true only for the case of pure strain but not for flows with mean vorticity. For three-dimensional flows in general, the measured flow distribution can be predicted only by choosing different viscosities for each stress component (Markatos 1987). Indeed, a complete derivation of equation (21a) indicates the presence of nonisotropic terms which break the "alignment assumption" and which ultimately are responsible for the extra terms discussed in (*b*) above. In other words, in lieu of equation (21a), one has (Taulbee 1992; Gatski & Speziale 1993)

$$b_{ij} \sim \nu_t S_{ij} + ab_{ik}S_{kj} + cb_{ik}\omega_{ik} + \cdots , \quad (21l)$$

where $2\omega_{ij} = U_{i,j} - U_{j,i}$ is the mean vorticity.

d. Equations (21a, b) imply that the Reynolds stress has contributions only from the shear and that the convective flux has contributions only from the temperature gradient. This is not correct, however. In principle,

$$b_{ij} \sim \sum_n (\text{shear terms} + \text{buoyancy terms})^n ,$$

$$\overline{u_i\theta} \sim \sum_n \left(\frac{\partial T}{\partial x_i} + \text{shear terms}\right)^n , \quad (21m)$$

where the summation begins with $n = 1$. At the lowest order, equations (21e)–(21f) become

$$\epsilon = \nu_t S^2(1 - R_f) , \quad \nu_t = (C_s\Delta)^2 S(1 - R_f)^{1/2} \quad (21n)$$

where R_f is the flux Richardson number, the ratio of the energy (more precisely the power) generated by buoyancy to that generated by shear (for the definition of λ_i, see after eq. [27c]:

$$R_f = \frac{\lambda_i \overline{u_i\theta}}{b_{jk}S_{jk}} . \quad (21o)$$

Since in unstably stratified regimes, $R_f < 0$, model (21f) *underestimates* the true turbulent viscosity, whereas in a stably stratified regime (like the overshooting region), $R_f > 0$, equation (21f) *overestimates* the true value of the turbulent viscosity.

e. Equation (21b) contradicts a well-known phenomenon observed in laboratory, atmospheric, and numerically simulated turbulence, namely that stably stratified flows exhibit both a positive temperature gradient and a positive convective flux:

$$\partial T/\partial z > 0 , \quad \overline{w\theta} > 0 , \quad (21p)$$

a phenomenon known as *countergradient* (Priestly & Swinbank 1947; Deardorff 1966; Finger & Schmidt 1986; Schumann 1987; Canuto et al. 1993). It will be shown later (see also Canuto 1992, eq. [80]) that one of the terms that contributes to the countergradient phenomenon and which is missing in equation (21b) is θ^2, the temperature variance.

f. Equation (21b) is not valid in stratified flows where the presence of strong θ^2 fluctuations (random gravity waves) forces the turbulent conductivity χ_t to become a tensor: this is shown explicitly in § 6, equation (49a).

g. Equation (21c) is taken with a constant turbulent Prandtl number σ_t. This contradicts experimental data (Webster 1964, Istweire & Helland 1989) which show that in stably stratified flows σ_t *increases* with increasing stability, indicating a more efficient transport of momentum than of heat.

h. Equation (21f) is based upon equations (21d) and (21e). Let us begin with the latter: it states that production equals dissipation, that is, turbulence is assumed to be in a state of local equilibrium; at each point in the flow, turbulent energy is dissipated at the same rate at which is produced, whereas the strong nonlocal nature of convection implies that turbulent energy generated at one point in the flow may be dissipated somewhere else (see, for example, Chan & Sofia 1989). The assumption of locality is contained in equation (21d).

The assumption of locality can be expected to apply to flows that are locally produced and locally dissipated. Shear turbulence is such a flow whereas convective turbulence is not, its most distinguishing feature being the high degree of nonlocality (Monin & Yaglom 1971–1975).

In summary, the premises under which the SGS model (21a)–(21f) is expected to hold are satisfied much more in shear turbulence than in convective turbulence. This conclusion is hardly surprising since the physical ingredients of the model were originally devised to describe shear rather than convective turbulence. Therefore, arguments (a)–(h) cast doubts as to the reliability of such an SGS model as a trustworthy description of turbulent convection. On the other hand, the general attitude has been to employ an "a posteriori" reasoning whereby the SGS model (21a)–(21f) is judged valid because by changing the values of the constants in it, the results do not change much. We do not concur with these conclusions, because the reasons given in (a)–(h) demonstrate that the physical content of the model is wanting in many respects, because one cannot quantify the importance of physical effects that the model does not include, because one should employ at least two SGS models of different physical content to make meaningful comparisons and because recent LES calculations have demonstrated that small scales can no longer be viewed as a pure drain of energy from the larger scales: they can in fact play a dynamical role by backscattering some of their energy to the larger scales, thus affecting the overall structure of the PBL (Mason & Thomson 1992).

5. THE COMPLETE MODEL

Following Deardorff (1970, 1971), Herring (1987), and Schmidt & Schumann (1989), *we assume that the SGS model for the Reynolds stress and fluxes (eq. [8]) is given by a SOC model.* Using the Reynolds stress approach to treat the Navier-Stokes equations (Papers I and II) and keeping buoyancy, shear, and rotation, one can derive the equations satisfied by the Reynolds stresses and the convective flux. We call (U_i, T) the resolved scales and (u_i, θ) the unresolved scales of the velocity and temperature fields. Also,

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + U_j \frac{\partial}{\partial x_j}, \quad b_{ij} = \overline{u_i u_j} - \frac{2}{3} e\,\delta_{ij}, \quad e \equiv \frac{1}{2}\overline{q^2}, \quad q^2 \equiv u_i u_i . \tag{22}$$

The derivation of the basic equations of the SGS model is presented in Appendix A. The results are as follows.

Turbulent kinetic energy e:

$$\frac{De}{Dt} + D_f(e) = -b_{ij} S_{ij} + \lambda_i \overline{u_i \theta} - \epsilon + \frac{1}{2} C_{ii} , \tag{23a}$$

where

$$D_f(e) \equiv \frac{\partial}{\partial x_i}\left(\frac{1}{2}\overline{q^2 u_i} + \overline{p u_i}\right) . \tag{23b}$$

Temperature variance $\overline{\theta^2}$:

$$\frac{D\overline{\theta^2}}{Dt} + D_f(\overline{\theta^2}) = -2\overline{u_i \theta}\frac{\partial T}{\partial x_i} + \chi \frac{\partial^2 \overline{\theta^2}}{\partial x_j^2} - 2\epsilon_\theta + C^\theta , \tag{24a}$$

where

$$D_f(\overline{\theta^2}) = \frac{\partial}{\partial x_i}\overline{u_i \theta^2} . \tag{24b}$$

Reynolds stresses b_{ij}:

$$\frac{D}{Dt} b_{ij} + D_f(b_{ij}) = -2c_4^* \tau_p^{-1} b_{ij} + \beta_5 B_{ij} - \frac{8}{15} e S_{ij} - (1-\alpha_1)\Sigma_{ij} - (1-\alpha_2) Z_{ij} - \Pi_{ij}(\mathrm{NL}) + C_{ij} - \frac{1}{3}\delta_{ij} C_{kk} , \tag{25a}$$

where

$$D_f(b_{ij}) = \frac{\partial}{\partial x_k}\left(\overline{u_i u_j u_k} - \frac{1}{3}\delta_{ij}\overline{q^2 u_k} + \delta_{ik}\overline{p u_j} + \delta_{jk}\overline{p u_i} - \frac{2}{3}\delta_{ij}\overline{p u_k}\right) \tag{25b}$$

Turbulent convective fluxes $F_c = c_p \rho \phi_i$, $\phi_i \equiv \overline{u_i \theta}$:

$$\frac{D}{Dt}\phi_i + D_f(\phi_i) = -\overline{u_i u_j}\frac{\partial T}{\partial x_j} - \left(1 - \frac{3}{4}\alpha_3\right) S_{ij}\phi_j - \left(1 - \frac{5}{4}\alpha_3\right)\Lambda_{ij}\phi_j - f_1 \tau_p^{-1}\phi_i + (1-\gamma_1)\lambda_i \overline{\theta^2} - \Pi_i^\theta(\mathrm{NL}) + \frac{1}{2}(\nu + \chi)\frac{\partial^2}{\partial x_j^2}\phi_i + C_i , \tag{26a}$$

where

$$D_f(\phi_i) = \frac{\partial}{\partial x_j}(\overline{\phi_i u_j} + \delta_{ij}\overline{p\theta}) . \tag{26b}$$

The functions D_f represent "diffusion terms" and are given by the third-order moments discussed in Appendix D.

Dissipation rates ϵ and ϵ_θ:

$$\epsilon = \frac{e^{3/2}}{l_\epsilon} , \quad \epsilon_\theta = \frac{1}{2} c_\theta \overline{\theta^2}\frac{\epsilon}{e} . \tag{27a}$$

For the dissipation length scale l_ϵ, we take

$$l_\epsilon = c_\epsilon^{-1} l , \quad l/\Delta = \Gamma(\mathrm{Fr}, R_f) , \quad c_\epsilon = \mathrm{const.} , \tag{27b}$$

where

$$\mathrm{Fr} = \frac{e^{1/2}}{\Delta N} , \quad R_f = \frac{\lambda_i \overline{u_i \theta}}{b_{ij} S_{ij}} , \quad N^2 = -\alpha g_i\left[\frac{\partial T}{\partial x_i} - \left(\frac{\partial T}{\partial x_i}\right)_{\mathrm{ad}}\right] \equiv \lambda_i \beta_i . \tag{27c}$$

Here Fr is the Froude number, R_f is the flux Richardson number, and N is the Brunt-Vaisala frequency ($N^2 > 0$ for unstable stratification and $N^2 < 0$ for stable stratification); $\lambda_i = g_i \alpha$, $g_i = (0, 0, g)$, where α is the volume expansion coefficient. Δ *is the limit of* l *in the neutral and shearless case.*

The function Γ has been computed by Cheng & Canuto (1993) with the result

$R_f < R_{fc}$:

$$\Gamma \equiv [1 + a\,\mathrm{Fr}^{-2}(1 + b\,\mathrm{Fr}^{-4/3})^{-1}]^{-3/2} , \quad 3\pi^2 a = 2(A - 1) , \quad b = 0.12|A - 1 + \tfrac{3}{2}A^{-1}|^{4/9} ; \tag{27d}$$

$R_f > R_{fc}$:

$$\Gamma \equiv [1 + (4/5\pi^2)A\,\mathrm{Fr}^{-2}]^c , \quad c = \tfrac{5}{4}(A^{-1} - 1) . \tag{27e}$$

In both expressions A is defined as

$$A \equiv 1 + (3^{1/2}/4)\mathrm{Ko}^{3/2}(R_{fc}/R_f - 1) \tag{27f}$$

Cheng & Canuto (1993) have also shown how the expression for l does encompass the empirical expressions suggested by Deardorff (1980) and Hunt et al. (1988).

The traceless tensors appearing in equations (23)–(27) are defined by

$$2S_{ij} = U_{i,j} + U_{j,i}\,, \quad 2\omega_{ij} = U_{i,j} - U_{j,i}\,,$$
$$B_{ij} = \lambda_i \phi_j + \lambda_j \phi_i - \tfrac{2}{3}\delta_{ij}\lambda_k \phi_k\,,$$
$$\Sigma_{ij} = S_{ik} b_{kj} + S_{jk} b_{ik} - \tfrac{2}{3}\delta_{ij} S_{kl} b_{kl}\,, \tag{28}$$
$$Z_{ij} \equiv b_{ik}\omega_{jk} + b_{jk}\omega_{ik} - (2-\alpha_2)(1-\alpha_2)^{-1}(\epsilon_{jkl} b_{ik} + \epsilon_{ikl} b_{jk})\Omega_l\,,$$
$$\Lambda_{ij} = \omega_{ij} - (2 - 5\alpha_3/4)(1 - 5\alpha_3/4)^{-1}\epsilon_{ijm}\Omega_m\,.$$

In equation (28), S_{ij} is the shear, ω_{ij} is the vorticity, Ω is the angular velocity, and ϵ_{ijk} is the totally antisymmetric tensor. From equation (25a) we note that B_{ij} represents a source of turbulence (specifically of b_{ij}) due to buoyancy, while Σ_{ij} and Z_{ij} represent "anisotropic production" of b_{ij} via the anisotropic interaction of the mean flow (S_{ik} and ω_{ik}) with the Reynolds stress b_{jk}. These terms are the ones that avoid the alignment problem discussed in item (*c*) of § 4.

The nonlinear quantities $\Pi_{ij}(\mathrm{NL})$ and $\Pi_i^\theta(\mathrm{NL})$ are given by equations (A27b)–(A29), (A41)–(A42) of Appendix A. The non-Boussinesq terms C_θ, C_i, and C_{ij} are derived in Appendix B. The third-order moments appearing on the left-hand sides of equations (23)–(26), are discussed in Appendix D. Finally, in Appendix E we present the expression of the functions β's and γ's and the values of the constants.

In summary, the complete model is composed of the differential equations (23)–(26) and of relations (27).

Since it would not seem advisable to go from the Smagorinsky model to the complete model, we present a hierarchy of simpler models so as to allow an orderly quantification of the new features of the full model.

6. ALGEBRAIC MODELS

If one neglects the convective and diffusive terms, represented by the left-hand sides of equations (23)–(26), these equations become algebraic and one can thus write the Reynolds stress tensor b_{ij} and the convective flux $\overline{u_i\theta}$ in a form that entails only inversion of matrices. This model was used, for example, by Launder (1975). Physically, this corresponds to assuming that production P equals dissipation ϵ, as is clear from equation (23), which becomes

$$P = \epsilon\,, \quad P \equiv P_b + P_s\,, \tag{29a}$$

where the buoyancy and shear production terms are defined by

$$P_b = \lambda_i \overline{u_i\theta}\,, \quad P_s = -b_{ij}S_{ij}\,. \tag{29b}$$

However, a better approximation can be devised that, while accounting for the possibility that locally $P \neq \epsilon$, still leads to an algebraic model (AM) which of course can easily be reduced to the previous case by taking $P/\epsilon = 1$. This approximation was originally suggested by Rodi (1984) and has been used extensively since then. We begin by considering equations (A23) and (A26), which we write in compact form as

$$\frac{D}{Dt}\overline{u_i u_j} + D_f(\overline{u_i u_j}) = \mathrm{RHS(A23)}\,, \tag{29c}$$

$$\frac{D}{Dt} e + D_f(e) = \mathrm{RHS(A26)}\,, \tag{29d}$$

where RHS(A23) and RHS(A26) mean the right-hand sides of equations (A23) and (A26), respectively. Introducing the dimensionless Reynolds stress tensor

$$a_{ij} = \frac{1}{e}\overline{u_i u_j} - \frac{2}{3}\delta_{ij} \equiv e^{-1} b_{ij}\,, \tag{30a}$$

equation (29c) becomes

$$e\frac{D}{Dt}a_{ij} + \frac{1}{e}\overline{u_i u_j}\left[\frac{De}{Dt} + D_f(e)\right] + \left[D_f(\overline{u_i u_j}) - \frac{1}{e}\overline{u_i u_j}D_f(e)\right] = \mathrm{RHS(A23)}\,. \tag{30b}$$

At this point, we employ Rodi's (1984) approximation whereby the diffusion of $\overline{u_i u_j}$ is assumed to be proportional to the diffusion of e with a coefficient given by the ratio $(\overline{u_i u_j}/e)$ which is not constant:

$$D_f(\overline{u_i u_j}) \approx (\overline{u_i u_j}/e)D_f(e) \tag{30c}$$

so that we can neglect the term in last set of brackets in the left-hand side of equation (30b). Furthermore, using equations (29d), (A23), and (A26), we derive

$$e\frac{D}{Dt}a_{ij} + a_{ij}\left(P - \epsilon + \frac{1}{2}C_{ii}\right) = -2c_4^* e\tau_p^{-1} a_{ij} - \frac{8}{15}eS_{ij} + \beta_5 B_{ij} - (1-\alpha_1)\Sigma_{ij} - (1-\alpha_2)Z_{ij} + C_{ij} - \frac{1}{3}\delta_{ij}C_{kk} - \Pi_{ij}(\mathrm{NL})\,. \tag{31}$$

Taulbee (1992) has recently shown that $Da_{ij}/Dt = 0$ holds true only in the asymptotic case, namely, for large values of the dimensionless parameter $\tau S \gg 1$, where τ is the characteristic time of turbulence, $\tau = 2e/\epsilon$, and S is the shear. It is clear that in many astrophysical settings of interest, for example in accretion disks, such a relation is not necessarily satisfied. Moreover, since the presence of buoyancy must also be accounted for, we extend Taulbee's suggestion by writing

$$S \to S_* = S(1 - R_f)^{1/2}\,, \tag{32a}$$

where the flux Richardson number is defined in equation (27c).

In order to encompass arbitrary values of τS_*, it is suggested that one introduces the variable $a_{ij}/\tau S_*$ and uses equation (C9) to eliminate the variable τ. Using an approximation analogous to equation (30c), equation (C9) becomes

$$\frac{1}{S_*}\frac{D}{Dt}(\tau S_*) = \frac{\tau}{S_*}\frac{D}{Dt}S_* + 2(C_{\epsilon_2} - 1) - 2(C_{\epsilon_1} - 1)\frac{P}{\epsilon} + \frac{1}{\epsilon}C_{ii}\,, \tag{32b}$$

where we have neglected the difference in the two diffusion terms.

Let us now consider equation (26). In this case, it has been suggested (Gibson & Launder 1976) that the left-hand side be taken as

$$\frac{D}{Dt}\overline{u_i\theta} + D_f(\overline{u_i\theta}) = \frac{1}{2}\overline{u_i\theta}\left[\frac{1}{e}\left(\frac{De}{Dt} + D_f e\right) + \frac{1}{\overline{\theta}^2}\left(\frac{D\overline{\theta}^2}{Dt} + D_f\overline{\theta}^2\right)\right], \tag{33a}$$

which, upon using equations (23)–(24), becomes

$$\frac{D}{Dt}\overline{u_i\theta} + D_f(\overline{u_i\theta}) = B\tau^{-1}\overline{u_i\theta}\,, \tag{33b}$$

where, using equations (29) and (27a)

$$P_\theta \equiv -\overline{u_i\theta}\frac{\partial T}{\partial x_i} + \frac{1}{2}C^\theta\,, \quad \tau_\theta = \frac{\overline{\theta^2}}{\epsilon_\theta} = \frac{2}{c_\theta}\,l_\epsilon e^{-1/2}\,, \tag{33c}$$

we obtain

$$B \equiv \frac{P}{\epsilon} - 1 + \frac{1}{2}\epsilon^{-1}C_{ii} + c_\theta\left(\frac{P_\theta}{\epsilon_\theta} - 1 + \mathrm{Pe}^{-1}\right), \tag{33d}$$

where we have introduced the Peclet number defined as

$$\mathrm{Pe} = c_\theta\,\frac{e^{1/2}}{\chi}\,l_\epsilon\left(\frac{l_\epsilon^2}{\overline{\theta^2}}\,\frac{\partial^2\overline{\theta^2}}{\partial x_j^2}\right)^{-1}. \tag{33e}$$

Substituting now equations (32b) with $D(a_{ij}/\tau S_*)/Dt = 0$ and equation (33b) into the left-hand sides of equations (31) and (26), we obtain the following.

6.1. *AM1: Two-Equation Model*

Reynolds stresses:

$$Ab_{ij} = -\tfrac{8}{15}e\tau S_{ij} + \beta_5\tau B_{ij} - (1-\alpha_1)\tau\Sigma_{ij} - (1-\alpha_2)\tau Z_{ij} + -\tau\Pi_{ij}(\mathrm{NL}) + \tau(C_{ij} - \tfrac{1}{3}\delta_{ij}C_{kk})\,, \tag{34a}$$

where

$$A \equiv A_0 + A_1\frac{P}{\epsilon} + \frac{2}{\epsilon}C_{ii} + \frac{\tau}{S_*}\frac{D}{Dt}S_*\,, \tag{34b}$$

$$\frac{1}{2}A_0 \equiv \frac{\tau}{\tau_p}c_4^* + C_{\epsilon_2} - 2\,, \quad \frac{1}{2}A_1 \equiv 2 - C_{\epsilon_1}\,. \tag{34c}$$

Convective fluxes:

$$A_{ik}\overline{u_k\theta} = -\left(\frac{2}{3}e\,\delta_{ij} + b_{ij}\right)\tau\frac{\partial T}{\partial x_j} + (1-\gamma_1)\lambda_i\tau\overline{\theta}^2 - \tau\Pi_i^\theta(\mathrm{NL}) + \frac{1}{2}\tau(\nu+\chi)\frac{\partial^2}{\partial x_j^2}\overline{u_i\theta} + \tau C_i\,, \tag{35a}$$

where

$$A_{ik} \equiv \left(\frac{\tau}{\tau_p}f_1 + B\right)\delta_{ik} + \left(1 - \frac{3}{4}\alpha_3\right)\tau S_{ik} + \left(1 - \frac{5}{4}\alpha_3\right)\tau\Lambda_{ik}\,. \tag{35b}$$

We may note several features of the general expressions (34a) and (35a). First of all, the ratio τ/τ_p is not a constant unless one deals with neutral stratification. Otherwise, the expression is

$$\frac{\tau}{\tau_p} = 1 + h|N^2|\tau^2\,, \quad h = 0.04\delta\,, \tag{35c}$$

where $\delta = 0$ for unstable stratification and $\delta = 1$ for stable stratification. Since $\tau = 2e^{-1/2}l_\epsilon$, we have

$$\frac{\tau}{\tau_p} = 1 + 4hl_\epsilon^2|N^2|e^{-1}\,. \tag{35d}$$

Equation (34a) shows that shear (S_{ij}) and buoyancy (B_{ij}) contribute to the Reynolds stresses as well as anisotropic production (Σ and Z), the non-Boussinesq terms (C), and the nonlinear terms (Δ and Π) which become important in the stably stratified region. Equation (34a) exhibits the general structure of equation (21l). By the same token, equation (35a) shows that buoyancy has contributions from not only the temperature gradient but also by shear and by temperature fluctuations $\overline{\theta^2}$.

In conclusion, the AM1 model consists of equations (23), (24), (27), (34), and (35). It is a two-equation model since there are only two differential equations (e, $\overline{\theta^2}$), while the remaining turbulent variables are expressed algebraically.

6.2. *AM2: One-Equation Model*

In this model, we carry out a further simplification: we change equation (24a) from prognostic to diagnostic by neglecting the time derivative and the third-order moments. Using equation (27a) and $\tau = 2e/\epsilon$, we obtain

$$\overline{\theta^2} = -\tau C_*^{-1}\left(\overline{u_i\theta}\,\frac{\partial T}{\partial x_i} - \frac{1}{2}C^\theta\right), \tag{36a}$$

which, together with the first term of equation (B6), gives

$$\overline{\theta^2} = -\tau C_*^{-1}\overline{u_i\theta}\left[\frac{\partial T}{\partial x_i} - \left(\frac{\partial T}{\partial x_i}\right)_{\mathrm{ad}}\right] = \tau C_*^{-1}\beta_i\overline{u_i\theta}\,, \tag{36b}$$

where (see eq. [27c])

$$\beta_i = -\left[\frac{\partial T}{\partial x_i} - \left(\frac{\partial T}{\partial x_i}\right)_{\mathrm{ad}}\right], \quad C_* \equiv c_\theta(1 + \mathrm{Pe}^{-1})\,. \tag{36c}$$

Thus, equation (35a) simplifies to

$$A_{ik}\overline{u_k\theta} = -\left(\frac{2}{3}e\,\delta_{ij} + b_{ij}\right)\tau\frac{\partial T}{\partial x_j} - \tau\Pi_i^\theta(\mathrm{NL}) + \tau C_i + \frac{1}{2}\tau(\nu+\chi)\frac{\partial^2}{\partial x_j^2}\overline{u_i\theta}\,, \tag{37a}$$

where the matrix A_{ik} is now given by

$$A_{ik} \equiv \left(\frac{\tau}{\tau_p}f_1 + B\right)\delta_{ik} - C_*^{-1}(1-\gamma_1)\tau^2\lambda_i\beta_k + \left(1 - \frac{3}{4}\alpha_3\right)\tau S_{ik} + \left(1 - \frac{5}{4}\alpha_3\right)\tau\Lambda_{ik}\,. \tag{37b}$$

Model AM2 is thus composed of equations (23), (27), (34), and (37). It is a one-equation model.

6.3. *AM3: One-Equation Model, Neglect of Higher Order Terms*

In this model, we further simplify the structure of the equations by neglecting the nonlinear contributions to the pressure correlations; namely, we assume that

$$\Pi_{ij}(\mathrm{NL})\,, \quad \Pi_i^\theta(\mathrm{NL}) = 0\,. \tag{38}$$

Thus we obtain from equation (34a) the following.

Reynolds stresses:

$$Ab_{ij} = -\tfrac{8}{15}e\tau S_{ij} + \beta_5\tau B_{ij} - (1-\alpha_1)\tau\Sigma_{ij} - (1-\alpha_2)\tau Z_{ij} + \tau(C_{ij} - \tfrac{1}{3}\delta_{ij}C_{kk}) \tag{39}$$

with A given by equations (34b)–(34c). By the same token, we derive from equation (37a) the following.

Convective fluxes:

$$A_{ik}\overline{u_k\theta} = -\left(\frac{2}{3}e\,\delta_{ij} + b_{ij}\right)\tau\frac{\partial T}{\partial x_j} + \tau C_i + \frac{1}{2}\tau(\nu+\chi)\frac{\partial^2}{\partial x_j^2}\overline{u_i\theta}\,, \tag{40}$$

with A_{ik} given by equation (37b). Model AM3 is thus composed of equations (23), (27), (39), and (40). It is a one-equation linear model.

6.4. *AM4: Zero-Equation Model*

In this model, we change the only remaining differential equation (eq. [23a]), from prognostic to diagnostic, thus reducing the model to a zero-equation model since all turbulent variables will now be given in algebraic form. Under these assumptions, equation (23a) becomes the statement that production equals dissipation:

$$\epsilon = -b_{ij} S_{ij} + \lambda_i \overline{u_i \theta} = -b_{ij} S_{ij}(1 - R_f) . \quad (41)$$

Thus model AM4 consists of equations (39), (40), and (41). It is a completely algebraic model with no differential equations (hence the name zero-equation model).

7. SIMPLIFIED MODELS

Clearly, all of the previous SGS models can easily be solved numerically but not analytically. To illustrate some of the main features, we shall present a class of simplified models (hence the name SM) that can be worked out more explicitly provided one neglects some of the terms in the expressions for b_{ij} and $\overline{u_i \theta}$. Since such simplifications may not be fully justified, the main purpose here is to fill the gap between the AM and the well-known Smagorinsky-Lilly model.

7.1. *SM1: Smagorinsky-Lilly Model*

This model is recovered from the previous expressions if one takes equations (39) and (40) to be of the form

$$b_{ij} = -2\nu_t S_{ij} , \quad (42a)$$

$$\overline{u_i \theta} = \chi_t \beta_i , \quad (42b)$$

which alone shows that such a model does not account for the production of b_{ij} due to buoyancy (B_{ij}), the anisotropic production of b_{ij} due to shear (Σ_{ij}), and the anisotropic production of b_{ij} due to vorticity (Z_{ij}). At the level of the convective flux, such a model neglects the anisotropic production due to the interaction of b_{ij} with the temperature gradient, the $\bar{\theta}^2$ fluctuations, shear, and vorticity contributions (the last three terms are part of A_{ik}; eq. [37b]). Since $\tau = 2e/\epsilon$ and ϵ is given by equation (27a), the expressions for ν_t and χ_t in equation (42) acquire the familar forms

$$\nu_t = c_\nu e^{1/2} l_\epsilon , \quad \chi_t = c_\chi e^{1/2} l_\epsilon . \quad (42c)$$

Once the kinetic energy e is obtained from solving equation (41), the final form for ν_t is

$$\nu_t = (C_s \Delta)^2 S[1 + \sigma_t^{-1}(0)\mathrm{Ri}]^{1/2} , \quad (42d)$$

where

$$C_s = c_\nu^{3/4} c_\epsilon^{-1} , \quad \sigma_t(0) = \nu_t \chi_t^{-1} = c_\nu c_\chi^{-1} , \quad \mathrm{Ri} = \frac{N^2}{S^2} . \quad (42e)$$

Here, C_s is the Smagorinsky constant, $\sigma_t(0)$ is the turbulent Prandtl number corresponding to neutral stratification, and Ri is the Richardson number. We recall that with the present definition of N^2, equations (27c) and (36c), we have

Unstable stratification:

$$N^2 > 0 , \quad \overline{u_i \theta} > 0 , \quad R_f < 0 ; \quad (43a)$$

Stable stratification:

$$N^2 < 0 , \quad \overline{u_i \theta} < 0 , \quad R_f > 0 . \quad (43b)$$

In equations (42c), the constants are given by

$$c_\nu = \frac{8}{15a} , \quad \frac{1}{2} a \equiv c_4^* + C_{\epsilon_2} - C_{\epsilon_1} , \quad (44a)$$

$$c_\chi \equiv \frac{4}{3}(f_1 + B)^{-1} . \quad (44b)$$

As for their numerical values, using the values given in Appendix E, we obtain ($F^{1/2} = 0.8$ and $F = 0$)

$$c_\nu = 0.096\text{–}0.112 . \quad (44c)$$

Schumann (1991) adopts $c_\nu = 0.072$, while Rodi (1984) suggests $c_\nu = 0.08$. With the value $f_1 = 7.5$, we obtain

$$c_\chi = 0.178 , \quad (44d)$$

while Schumann (1991) uses the value of 0.172. Finally (with $c_\epsilon = 0.845$, Appendix C),

$$0.54 < \sigma_t(0) < 0.63 , \quad (44e)$$

$$0.20 \le C_s \le 0.23 . \quad (44f)$$

This value of C_s is very close to the original value first derived by Lilly (1962, 1966, 1967).

7.2. *SM2: Reynolds Stresses*

The Smagorinsky-Lilly model does not account for any of the four effects

$$\theta^2\text{-fluctuations} , \quad \tau_p \neq \tau , \quad l \neq \Delta , \quad S_* , \quad (45)$$

i.e., the influence of θ^2-fluctuations, the shortening of the pressure-velocity correlation timescale, the effect of stratification and shear on the dissipation length scale, and the dynamic effects due to S_*. Below, we present a set of models that account for equation (45) while of course making other approximations so as to make the models tractable.

Without any justification other than simplicity, we take

$$b_{ij} = -2\nu_t S_{ij} . \quad (46)$$

The effect of τ_p and S_* contained in equations (34b)–(34c) gives rise to an expression for ν_t different than equation (42c). In fact, we now have

$$\nu_t = c_\nu e^{1/2} l_\epsilon \Phi_1(e) , \quad (47a)$$

where

$$\Phi_1(e) \equiv \left[1 + b\left(\frac{l_\epsilon^2 |N^2|}{e}\right) + c\left(\frac{l_\epsilon S}{e^{1/2}}\right)\right]^{-1} , \quad (47b)$$

$$b \equiv 8c_4^* h a^{-1} \approx 4h , \quad c \equiv 2a^{-1}\Sigma_b , \quad (47c)$$

$$\Sigma_b \equiv \Sigma - \frac{1}{2}(1 - R_f)^{-1} S^{-1} \frac{D}{Dt} R_f , \quad \Sigma \equiv S^{-2} \frac{DS}{Dt} . \quad (47d)$$

Substituting equation (47a) into equation (41) and using equation (27a), we obtain the equation determining the kinematic energy e, namely,

$$e(l_\epsilon S)^{-2} = c_\nu(1 - R_f)\Phi_1(e) . \quad (48a)$$

To solve this equation, one needs to know R_f as a function of e itself and this in turn requires a model for the convective flux.

In fact,

$$R_f = \frac{\lambda_i \overline{u_i \theta}}{b_{ij} S_{ij}} = -\lambda_i \overline{u_i \theta}(\nu_t S^2)^{-1} . \tag{48b}$$

An alternative form for R_f comes from using equation (41), namely,

$$R_f(1 - R_f)^{-1} = -l_\epsilon e^{-3/2} \lambda_i \overline{u_i \theta} . \tag{48c}$$

We should also recall that l_ϵ itself is a function of e because of equations (27b)–(27f). Once the kinetic energy e is known in terms of the large-scale quantities, the turbulent viscosity ν_t is computed from equation (47a).

7.3. *Turbulent Convective Flux*

The convective flux, which in principle is given by equation (40), will be simplified by neglecting the anisotropy factor b_{ij} on the right-hand side as well as the influence of shear and vorticity in equation (37b). Even so, the derivation of the expression for the convective flux is by no means simple due to the presence of the $\overline{\theta^2}$ fluctuations which introduce the non-diagonal term $\lambda_i \beta_k$ in equation (37b). Application of matrix algebra and in particular the Cayley-Hamilton theorem yields the result

$$\overline{u_i \theta} = \chi^t_{ij} \beta_j , \tag{49a}$$

where the *turbulent conductivity* is now a tensor χ^t_{ij} given by

$$\chi^t_{ij} = c_\chi e^{1/2} l_\epsilon \left[1 + d\left(\frac{l_\epsilon^2 |N^2|}{e}\right)\right]^{-1} [\delta_{ij} + L_{ij} + \Lambda L_{ik} L_{kj}] , \tag{49b}$$

with

$$L_{ij} = c_2 \left[1 + d\left(\frac{l_\epsilon^2 |N^2|}{e}\right)\right]^{-1} \frac{l_\epsilon^2}{e} \lambda_i \beta_j , \tag{49c}$$

$$\Lambda^{-1} \equiv 1 - c_2 \left[1 + d\left(\frac{l_\epsilon^2 |N^2|}{e}\right)\right]^{-1} \frac{l_\epsilon^2 N^2}{e} , \tag{49d}$$

where the constants are defined as follows

$$d \equiv 4hf \approx 4h = b , \quad f \equiv f_1(f_1 + B)^{-1} , \quad c_2 \equiv \frac{3}{C_*}(1 - \gamma_1)c_\chi . \tag{49e}$$

In equation (49b), the first bracket is due to the difference between τ_p and τ, while the second bracket is due to the presence of $\overline{\theta^2}$ fluctuations. After some algebra, we derive the expression needed to compute the flux Richardson number, namely,

$$\lambda_i \overline{u_i \theta} = c_\chi e^{1/2} l_\epsilon N^2 \Phi_2(e) , \tag{50a}$$

where

$$\Phi_2(e) \equiv \phi \frac{1 - c_2' l_\epsilon^2 e^{-1} N^2 \phi}{1 - c_2 l_\epsilon^2 e^{-1} N^2 \phi} , \tag{50b}$$

$$\phi^{-1} \equiv 1 + d\left(\frac{l_\epsilon^2 |N^2|}{e}\right) , \quad c_2' = c_2(1 - \lambda^2 \beta^2 N^{-4}) . \tag{50c}$$

We recall that the presence of c_2 is due to the $\overline{\theta^2}$ fluctuations, while ϕ is due to the fact that in general $\tau_p \neq \tau$. The remaining variables are defined as follows:

$$\beta^2 \equiv \beta_j \beta_j , \quad \lambda^2 = \lambda_j \lambda_j , \quad N^2 = \lambda_i \beta_i . \tag{50d}$$

In laboratory settings, where the temperature gradient typically has only one component,

$$\beta^2 \lambda^2 = N^4 . \tag{50e}$$

On the other hand, in a SGS model, equation (50e) is no longer true since β_i has all three components different from zero. Using equations (42a) and (42c), we finally obtain the expression for R_f as a function of the kinetic energy e, namely,

$$R_f = -\sigma_t^{-1}(0) \Phi_2(e) \Phi_1^{-1}(e) N^2 S^{-2} . \tag{51a}$$

Equation (51a) is now substituted into equation (48a) with the result

$$\frac{e}{l_\epsilon^2 S^2} = c_\nu [\Phi_1(e) + \sigma_t^{-1}(0) N^2 S^{-2} \Phi_2(e)] . \tag{51b}$$

At this point, one must use equations (27b)–(27f) for l_ϵ in general is a function of e. Once that is done, the solution of equation (51b) finally yields the desired relation

$$e = e(N, S) , \tag{51c}$$

and so *all the SGS variables are now known in terms of the large-scale variables, as desired.*

In summary, SM2 is an algebraic model given by the following relations

$$b_{ij} = -2\nu_t S_{ij} , \tag{52a}$$

$$\nu_t = \Delta e^{1/2} S_m , \tag{52b}$$

$$S_m = c_\nu c_\epsilon^{-1} \Gamma \Phi_1 , \tag{52c}$$

where Γ is a function of both shear and buoyancy given by equations (27d)–(27f); Φ_1 is given by equation (47b) and it accounts for the possibility that $\tau_p \neq \tau$. Similarly,

$$\lambda_i \overline{u_i \theta} = \chi_t N^2 , \tag{53a}$$

where N^2 is defined in equation (27c) and

$$\chi_t = \Delta e^{1/2} S_H , \tag{53b}$$

$$S_H = c_\chi c_\epsilon^{-1} \Gamma \Phi_2 , \tag{52c}$$

where Φ_2 is given by equations (50b)–(50c) and it accounts for the θ^2 fluctuations and $\tau_p \neq \tau$. Finally, the kinetic energy e is obtained by solving equation (51b).

7.4. *SM3: No Stratification, the Effect of Σ Alone*

Suppose we treat a case with no stratification, in which case $\mathrm{Ri} \to 0$ and $\Phi_2 \to 1$. Equation (51b) then yields

$$\frac{e^{1/2}}{l_\epsilon S} = c_\nu^{1/2}([1 + \mu^2 \Sigma^2]^{1/2} - \mu\Sigma) , \tag{54a}$$

where

$$\mu = \frac{15}{8} c_\nu^{1/2} , \quad \Sigma = S^{-2} \frac{DS}{Dt} . \tag{54b}$$

Since we want to study the effect of Σ, we take

$$l_c = c_\epsilon^{-1} l , \quad l = \Delta , \quad \Gamma = 1 . \tag{55a}$$

Substitution of equation (54) into equation (47a) yields

$$\nu_t = (C_s \Delta)^2 S \Psi_1(\Sigma) , \tag{55b}$$

where

$$\Psi_1(\Sigma) = ([1 + \mu^2\Sigma^2]^{1/2} + \mu\Sigma)^{-3} . \quad (55c)$$

The interesting new feature is the appearance of the dynamical variable Σ. We notice that for positive Σ, equation (55b) implies a *less dissipative* model since

$$\nu_t(\Sigma) < \nu_t(0) . \quad (55d)$$

This result is in contrast with a recent work by Yoshizawa (1989), who has derived

$$\Psi_1(\Sigma) = (1 + 0.64\Sigma)^2 , \quad (55e)$$

which implies that for positive Σ

$$\nu_t(\Sigma) > \nu_t(0) \quad (55f)$$

and thus a *more dissipative* model. It must be noted, however, that preliminary LES calculations show that the presence of Σ may be important only in unsteady flows.

7.5. *SM4: No Stratification, Effect of Shear on the Smagorinsky Constant*

In this case we take $\Sigma = 0$, but use $l_\epsilon = c_\epsilon^{-1}\Delta\Gamma$. For $N^2 \to 0$, equations (27d)–(27f) give

$$\Gamma = (1 + p\mathrm{Sh}^2)^{-3/2} , \quad p \equiv (2\pi^2 3^{1/2})^{-1}\mathrm{Ko}^{3/2} R_{fc}\,\sigma_t(0) . \quad (56a)$$

Substituting equation (56a) into equation (51b), we obtain

$$x^3 + 3x^2 - (m - 3)x + 1 = 0 , \quad (56b)$$

$$x \equiv p\mathrm{Sh}^2 , \quad m \equiv c_\nu(pc_\epsilon^2)^{-1} \quad (56c)$$

so that

$$\nu_t = (\tilde{C}_s\Delta)^2 S , \quad (56d)$$

where

$$\tilde{C}_s = C_s(1 + x)^{-3/2} . \quad (56e)$$

Solving equation (56b), we obtain the values in Table 1.

There are no real solutions for larger values of p. For example, for the last value of p and $\mathrm{Ko} = 1.6$, we have

$$R_{fc}\,\sigma_t(0) = 0.4 , \quad (56f)$$

$$0.45 \le \tilde{C}_s/C_s \le 0.63 . \quad (56g)$$

Thus, the effective Smagorinsky constant is reduced to about half Lilly's original value. Since $C_s = 0.2$, it follows that

$$\tilde{C}_s = 0.1 , \quad (56h)$$

which is indeed the value that Deardorff (1970) found was necessary to fit channel flow data. We can therefore conclude that the physical reason for the lowering of the Smagorinsky constant is the effect of shear. Let us further note that for $\sigma_t(0) = 0.72$ (Yakhot & Orszag 1986), equation (56f) yields $R_{fc} = 0.55$ which is a value frequently used.

TABLE 1

EFFECT OF SHEAR ON THE SMAGORINSKY CONSTANT

10^2p	$\tilde{C}_s/C_s$
2.0...........	0.33–0.75
2.4...........	0.45–0.63

7.6. *SM5: Stable and Unstable Stratification, The Effect of $\overline{\theta^2}$ and τ_p*

In this case we want to study the effect of $\overline{\theta^2}$ and τ_p separately from that of Γ; thus, we take

$$\Gamma = 1 , \quad l_\epsilon = c_\epsilon^{-1}\Delta , \quad c = 0 . \quad (57a)$$

Solving equation (51b), we obtain the *turbulent kinetic energy*:

$$\frac{e}{\Delta^2 S^2} = c_\nu c_\epsilon^{-2} y(\mathrm{Ri}) , \quad (58a)$$

$$y(\mathrm{Ri}) = \tfrac{1}{2} + \tfrac{1}{2}[1 + 4p\,\mathrm{Ri}^2\sigma_t^{-2}(0)]^{1/2} + \mathrm{Ri}\,\sigma_t^{-1}(0) - bc_\nu^{-1}|\mathrm{Ri}| , \quad (58b)$$

$$p \equiv \beta^2\lambda^2 N^{-4} . \quad (58c)$$

Equation (58b) can be compared with the standard expression, equations (42c)–(42d),

$$y(\mathrm{Ri}) = 1 + \mathrm{Ri}\,\sigma_t^{-1}(0) . \quad (58d)$$

Equation (58b) includes the contributions of both $\overline{\theta^2}$ and τ_p, whereas the standard expression (58d) contains neither. We must note that in deriving equation (58b) we have assumed $c_2 = c_\chi$, which corresponds to taking $c_\theta = C_* = 2$ and $\gamma_1 = \frac{1}{3}$, see equations (36c), (44b), and (E13).

Using equation (51a), we define the turbulent Prandtl number $\sigma_t(\mathrm{Ri})$ as

$$R_f = -\mathrm{Ri}\,\sigma_t^{-1}(\mathrm{Ri}) . \quad (59a)$$

Since σ_t is always positive, and $\mathrm{Ri} < 0$ for stable stratification, equation (59a) implies $R_f > 0$ for stable stratification, which is physically correct. Thus, we derive the *turbulent Prandtl number* $\sigma_t(\mathrm{Ri})$:

$$\sigma_t(\mathrm{Ri})/\sigma_t(0) = (1 + Ay^{-1}\mathrm{Ri})(1 + By^{-1}\mathrm{Ri})^{-1} , \quad (59b)$$

where

$$A \equiv c_\nu^{-1}(b \operatorname{sgn} \mathrm{Ri} - c_\chi) , \quad B \equiv c_\nu^{-1}[b \operatorname{sgn} \mathrm{Ri} - c_\chi(1 - p)] . \quad (59c)$$

Let us note that without the θ^2-contribution, $c_\chi = 0$, $A = B$, and so

$$\sigma_t(\mathrm{Ri})/\sigma_t(0) = 1 , \quad (59c)$$

which is incorrect for stable stratification since $\sigma_t(\mathrm{Ri})$ is experimentally known to increase with Ri (Webster 1964).

Finally, from equation (47a) we derive the *turbulent viscosity*:

$$\nu_t = (C_s\Delta)^2 S y^{1/2}(1 + by^{-1}|\mathrm{Ri}|/c_\nu)^{-1} , \quad (60a)$$

$$C_s = c_\nu^{3/4} c_\epsilon^{-1} , \quad (60b)$$

to be compared with the standard expression, equation (42d),

$$\nu_t = (C_s\Delta)^2 S[1 + \mathrm{Ri}\,\sigma_t^{-1}(0)]^{1/2} , \quad (60c)$$

to which equation (60a) reduces if $\theta^2 \to 0$ and $\tau_p = \tau$.

Finally, the turbulent conductivity χ_t is obtained from

$$\chi_t = \nu_t\sigma_t^{-1}(\mathrm{Ri}) , \quad (61a)$$

where $\nu_t(\mathrm{Ri})$ and $\sigma_t(\mathrm{Ri})$ are given by equation (60a) and (59b). Equation (61a) must be compared with the standard expression, equation (42e),

$$\chi_t = \nu_t\sigma_t^{-1}(0) , \quad (61b)$$

where ν_t is given by equation (60c).

7.6.1. *Stable Stratification:* $\mathrm{Ri} < 0$

In Tables 2 and 3 we display the solutions of equation (60c), called ν_t(standard) and equation (60a) versus Ri. The units of ν_t are $(C_s\Delta)^2 S$.

TABLE 2

ν_t: Effect of θ^2 Fluctuations Only

$-$Ri	ν_t(standard)	ν_t
0.............	1	1
0.1...........	0.92	0.93
0.2...........	0.82	0.88
0.3...........	0.72	0.84
0.4...........	0.59	0.82

The inclusion of θ^2 alone in Table 2 *increases* the standard turbulent viscosity ν_t: for example, in terms of the Smagorinsky constant C_s, at $-\mathrm{Ri} = 0.4$, this amounts to an *increase of* C_s of about 18%. In Table 3, the inclusion of both θ^2 and $\tau_p \neq \tau$ implies a *decrease of* C_s. At $-\mathrm{Ri} = 0.4$, it corresponds to 74%.

The standard model (Table 4) yields $\sigma_t(\mathrm{Ri})/\sigma_t(0) = 1$. In addition, the reason why there is only one case is because there is no effect of $\tau_p \neq \tau$ on σ_t. The increase of the ratio $\sigma_t(\mathrm{Ri})/\sigma_t(0)$ is in qualitative and quantitative accord with both experimental data (Webster 1964) and numerical simulations (Gerz, Schumann, & Elghobashi 1989, Fig. 8).

Next, we consider χ_t given by equations (61a) and (61b). Using the previous results, we obtain the values presented in Tables 5 and 6 (the units of χ_t are $\sigma_t^{-1}(0)(C_s\Delta)^2S$). As for χ_t, we notice that both θ^2 and $\tau_p \neq \tau$ have the effect of lowering χ_t versus the standard value: for example, at $-\mathrm{Ri} = 0.4$, the first effect corresponds to a decrease of C_s of about 15%, whereas the addition of the $\tau_p \neq \tau$ effect leads to a decrease of C_s about 80%. The decrease of χ_t due to θ^2 can be understood when we recall that physically

$$\overline{w\theta} = -\chi_t \frac{\partial T}{\partial z} + c_1\overline{\theta^2} . \tag{62a}$$

Since θ^2 is a positive contribution to a negative convective flux ($\partial T/\partial z > 0$), θ^2 acts like a countergradient; namely, we can write

$$\overline{w\theta} = -(\chi_t - \chi_t^{\theta}) \frac{\partial T}{\partial z} \equiv -\chi_t^{\mathrm{eff}} \frac{\partial T}{\partial z} \tag{62b}$$

with

$$\chi_t^{\mathrm{eff}} < \chi_t . \tag{62c}$$

TABLE 3

ν_t: Effect of θ^2 Fluctuations and of $\tau_p \neq \tau$

$-$Ri	ν_t(standard)	ν_t
0.............	1	1
0.1...........	0.92	0.70
0.2...........	0.82	0.43
0.3...........	0.72	0.20
0.4...........	0.59	0.04

TABLE 4

$\sigma_t(\mathrm{Ri})/\sigma_t(0)$ vs. Ri: Equation (59b)

$-$Ri	$\sigma_t(\mathrm{Ri})/\sigma_t(0)$
0....................	1
0.1..................	1.19
0.2..................	1.42
0.3..................	1.68
0.4..................	1.97

TABLE 5

χ_t: Effect of θ^2 Fluctuations

$-$Ri	χ_t(standard)	χ_t
0.............	1	1
0.1...........	0.92	0.78
0.2...........	0.82	0.62
0.3...........	0.72	0.50
0.4...........	0.59	0.42

TABLE 6

χ_t: Effect of θ^2 Fluctuations and of $\tau_p \neq \tau$

$-$Ri	χ_t(standard)	χ_t
0.............	1	1
0.1...........	0.92	0.63
0.2...........	0.82	0.30
0.3...........	0.72	0.12
0.4...........	0.59	0.02

7.6.2. *Unstable Stratification:* Ri > 0

In this case, we have only one effect, that of the θ^2 fluctuations since $\tau_p = \tau$. Using the previous expressions, we obtain the results in Table 7. Thus, the effect of the θ^2 fluctuations is to enhance the value of the turbulent viscosity with respect to the standard case. Analogously, for χ_t we derive the results in Table 8. As before, the inclusion of the θ^2 fluctuations enhances the value of χ_t.

It may be of interest to compare the previous results with those obtained with one of the empirical expressions often used in stably stratified turbulence (Pacanowski & Philander 1981; Smith & Hess 1993; due to the different definition of Ri in our work, we insert an absolute value),

$$\nu_t = \nu_t(0)(1 + \alpha|\mathrm{Ri}|)^{-n} , \quad \sigma_t = \sigma_t(0)(1 + \alpha|\mathrm{Ri}|) . \tag{62}$$

The linear dependence on Ri exhibited by the turbulent Prandtl number, equation (62), is not in agreement with the data of Gerz et al. (1989), whereas the values of Table 4 are. For

TABLE 7

ν_t: Effect of θ^2 Fluctuations

Ri	ν_t(standard)	ν_t
0.............	1	1
0.1...........	1.08	1.09
0.2...........	1.15	1.19
0.3...........	1.22	1.30
0.4...........	1.28	1.40

TABLE 8

χ_t: Effect of θ^2 Fluctuations

Ri	χ_t(standard)	χ_t
0.............	1	1
0.1...........	1.08	1.26
0.2...........	1.15	1.54
0.3...........	1.22	1.82
0.4...........	1.28	2.09

TABLE 9

ν_t AND σ_t FROM EQUATION (62) WITH $\alpha = 5$, $n = 2$

$-$Ri	ν_t	σ_t
0.............	1	1
0.1...........	0.44	1.5
0.2...........	0.25	2
0.3...........	0.16	2.5
0.4...........	0.11	3

example, at $|\mathrm{Ri}| = 0.4$, our result is 1.97, the data are around 2, while equation (62) predicts a value of 3 (Table 9).

8. CONCLUSIONS

Future turbulence research is likely to rely ever more heavily on large eddy simulations, an approach that has been exploited by geophysicists (and by the engineering community), who have made considerable progress in the understanding of the convective planetary boundary layer. LES techniques are viewed as "a potent technique of numerical calculation where measurements are difficult to obtain" (McWilliams et al. 1991). There is no reason why this philosophy should not be equally successful in astrophysics. Indeed, the LES results of an astrophysical nature presently available confirm such expectations even though the SGS models used thus far do not account for buoyancy, rotation, and stable stratification, whose inclusion is however essential. Astrophysical LES employ the Smagorinsky model (or even simpler models), which implies drastic approximations to the complete equations. Indeed, it is the most stripped-down version of the full model. It would thus seem logical to begin a "reverse trip" so as to include incrementally more physics into the SGS model. The hierarchy of SGS models we have derived is not the only possible one, however. Other combinations of the basic ingredients of the full model can be thought of to highlight a specific feature, e.g., rotation.

Although the hope is that one day the complete model, equations (22)–(28), will be implemented into the LES codes, the first logical candidates are the SM, followed by the AM, and finally by the complete model, CM. In all cases, the dissipation length scale l_ϵ is given by equations (27).

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APPENDIX A

A1. THE BASIC EQUATIONS

The basic equations describing a compressible fluid of total density $\tilde{\rho}$, pressure $\tilde{p}$, temperature $\tilde{T}$, velocity v_i, kinematic viscosity ν, and thermal conductivity K are given by ($d/dt \equiv \partial/\partial t + v_j \partial/\partial x_j$):

$$\tilde{\rho}\,\frac{d}{dt}\,v_i = -\frac{\partial \tilde{p}}{\partial x_i} - g_i \tilde{\rho} + \nu\tilde{\rho}\,\frac{\partial^2}{\partial x_j^2}\,v_i - 2\tilde{\rho}\epsilon_{ijk}\Omega_j v_k\,, \tag{A1}$$

$$\tilde{\rho}c_p\,\frac{d\tilde{T}}{dt} = \frac{d\tilde{p}}{dt} + K\,\frac{\partial^2 \tilde{T}}{\partial x_j^2} + \mu\left[\frac{\partial^2}{\partial x_i \partial x_j}\,v_i v_j + \left(\frac{\partial v_i}{\partial x_j}\right)^2\right] + c_p\tilde{\rho}Q\,, \tag{A2}$$

where $c_p\tilde{\rho}Q$ is the gradient of an external flux, $\mu = \tilde{\rho}\nu$, ϵ_{ijk} is the antisymmetric tensor, and Ω is the angular velocity. In addition, we assume a perfect gas law $\tilde{p} = R\tilde{\rho}\tilde{T}$. First, we split the variables into an average and a fluctuating part

$$\tilde{p} = P + p\,, \qquad \tilde{T} = T + \theta\,, \qquad \tilde{\rho} = \rho + \rho'\,, \qquad v_i = U_i + u_i\,, \tag{A3}$$

where P, T, ρ, and U_i represent the average fields; the fluctuating components have zero average

$$\bar{p} = \bar{\theta} = \overline{\rho'} = \bar{u}_i = 0\,. \tag{A4}$$

Assuming further that $P = R\rho T$, and neglecting second-order quantities, we derive for ρ' the relation

$$\frac{\rho'}{\rho} = -\alpha\theta + \frac{p}{P}\,, \qquad \alpha \equiv \frac{1}{T}\,. \tag{A5}$$

In the standard Boussinesq approximation (Paper I, eq. [21b]), the second term with the fluctuating pressure p/P is absent. The physical interpretation of the terms arising from its inclusion will be discussed shortly. Inserting equations (A3)–(A5) into equations (A1)–(A2), and following the procedures outlined in Paper I, we obtain the dynamical equations for the mean and fluctuating variables ($D/Dt \equiv \partial/\partial t + U_i \partial/\partial x_i$, $\lambda_i = g_i \alpha$, $g_i = 0, 0, g$; for any variable a, $a_{i,j} \equiv \partial a_i/\partial x_j$):

$$\frac{DU_i}{Dt} = -\left(g_i + \frac{1}{\rho}\frac{\partial P}{\partial x_i}\right) - \frac{\partial}{\partial x_j}\,\overline{u_i u_j} + N_1^i - 2\epsilon_{ijk}\Omega_j U_k\,, \tag{A6}$$

$$\frac{Du_i}{Dt} = -u_j\,\frac{\partial U_i}{\partial x_j} - \frac{\partial p}{\partial x_i} - \frac{\partial}{\partial x_j}\,(u_i u_j - \overline{u_i u_j}) + \lambda_i\theta + \nu\,\frac{\partial^2 u_i}{\partial x_j^2} + N_2^i - 2\epsilon_{ijk}\Omega_j u_k\,, \tag{A7}$$

$$\frac{DT}{Dt} = \chi\,\frac{\partial^2 T}{\partial x_j^2} - \frac{\partial}{\partial x_j}\,\overline{u_j\theta} + \frac{\epsilon}{c_p} + \frac{1}{c_p}\,U_j\,\frac{\partial P}{\partial x_j} + Q + N_3\,, \tag{A8}$$

$$\frac{D\theta}{Dt} = -u_j\,\frac{\partial T}{\partial x_j} - \frac{\partial}{\partial x_j}\,(u_j\theta - \overline{u_j\theta}) + \chi\,\frac{\partial^2\theta}{\partial x_j^2} + \frac{\nu}{c_p}\,[(u_{i,j})^2 - \overline{(u_{i,j})^2}] + N_4\,, \tag{A9}$$

where we have taken the $\nu \to 0$ limit and where ϵ is the dissipation rate of kinetic energy. The non-Boussinesq terms' Ns are given by (Paper II, eqs. [28]–[33])

$$\rho N_1^i \equiv -\alpha \overline{\theta \frac{\partial p}{\partial x_i}} + \overline{\frac{p}{P} \frac{\partial p}{\partial x_i}}, \tag{A10}$$

$$N_2^i \equiv -\left(g_i + \frac{1}{\rho}\frac{\partial P}{\partial x_i}\right)\alpha\rho\theta + \frac{p}{P}\frac{\partial P}{\partial x_i} - \alpha\left(\theta \frac{\partial p}{\partial x_i} - \overline{\theta \frac{\partial p}{\partial x_i}}\right) + \frac{1}{P}\left(p \frac{\partial p}{\partial x_i} - \overline{p \frac{\partial p}{\partial x_i}}\right), \tag{A11}$$

$$\rho c_p N_3 \equiv U_j \Lambda_j + \overline{u_j \frac{\partial p}{\partial x_j}} + \left(\alpha\overline{\theta u_j} - \frac{1}{P}\overline{p u_j}\right)\frac{\partial P}{\partial x_j} + \alpha\overline{\theta u_j \frac{\partial p}{\partial x_j}} - \frac{1}{P}\overline{p u_j \frac{\partial p}{\partial x_j}}, \tag{A12}$$

with

$$\Lambda_j \equiv \alpha\overline{\theta \frac{\partial p}{\partial x_j}} - \frac{1}{P}\overline{p \frac{\partial p}{\partial x_j}}, \tag{A13}$$

$$\begin{aligned} c_p \rho N_4 \equiv{}& U_j \Delta_j + u_j \frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_j}(p u_j - \overline{p u_j}) + \left[\alpha(\theta u_i - \overline{\theta u_i}) - \frac{1}{P}(p u_i - \overline{p u_i})\right]\frac{\partial P}{\partial x_i} \\ &+ \alpha\left(u_i \theta \frac{\partial p}{\partial x_i} - \overline{u_i \theta \frac{\partial p}{\partial x_i}}\right) - \frac{1}{P}\left(u_i p \frac{\partial p}{\partial x_i} - \overline{u_i p \frac{\partial p}{\partial x_i}}\right), \end{aligned} \tag{A14}$$

with

$$\Delta_i \equiv \frac{\partial p}{\partial x_i} - \left(\frac{p}{P} - \alpha\theta\right)\frac{\partial P}{\partial x_i} + \alpha\left(\theta \frac{\partial p}{\partial x_i} - \overline{\theta \frac{\partial p}{\partial x_i}}\right) - \frac{1}{P}\left(p \frac{\partial p}{\partial x_i} - \overline{p \frac{\partial p}{\partial x_i}}\right). \tag{A15}$$

A2. SECOND-ORDER MOMENTS

Following the procedure outlined in Papers I–II, we derive the following results:

$$\frac{D}{Dt}\overline{u_i\theta} + \frac{\partial}{\partial x_j}\overline{\theta u_i u_j} = -\left(\overline{u_i u_j}\frac{\partial T}{\partial x_j} + \overline{u_j \theta}\frac{\partial U_i}{\partial x_j}\right) + \lambda_i \overline{\theta^2} - \Pi_i^\theta + \eta_i - 2\epsilon_{ijk}\Omega_j \overline{u_k \theta} + C_i, \tag{A16}$$

where the pressure correlation term is defined as

$$\Pi_i^\theta \equiv \overline{\theta \frac{\partial p}{\partial x_i}} \tag{A17}$$

and the new term C_i is defined by

$$C_i \equiv \overline{N_2^i \theta} + \rho \overline{N_4 u_i} + \frac{\rho}{c_p}\overline{u_i \epsilon} \tag{A18}$$

with (Paper I, eq. [37f])

$$\overline{u_i \epsilon} = \tau^{-1}\overline{q^2 u_i}. \tag{A19}$$

Next, consider the equation for the temperature variance $\overline{\theta^2}$. In lieu of Paper I, equation (35a), we have

$$\frac{D\overline{\theta^2}}{Dt} + \frac{\partial}{\partial x_i}\overline{u_i \theta^2} = -2\overline{u_i \theta}\frac{\partial T}{\partial x_i} + \chi \frac{\partial^2 \overline{\theta^2}}{\partial x_j^2} - 2\epsilon_\theta + C^\theta, \tag{A20}$$

where

$$\frac{1}{2}C^\theta \equiv \overline{N_4 \theta} + \frac{1}{c_p}\overline{\epsilon\theta} \tag{A21}$$

with (Paper I, eq. [38e])

$$\overline{\epsilon\theta} = \tau^{-1}\overline{q^2\theta}. \tag{A22}$$

Next, consider the equation for the Reynolds stress $\overline{u_i u_j}$. We derive

$$\frac{D}{Dt}\overline{u_i u_j} + \frac{\partial}{\partial x_k}\overline{u_i u_j u_k} = -\left(\overline{u_j u_k}\frac{\partial U_i}{\partial x_k} + \overline{u_i u_k}\frac{\partial U_j}{\partial x_k}\right) + \lambda_i \overline{u_j \theta} + \lambda_j \overline{u_i \theta} - \Pi_{ij} + \nu \frac{\partial^2}{\partial x_k^2}\overline{u_i u_j} - \epsilon_{ij} - 2\Omega_{ij} + C_{ij}, \tag{A23}$$

where we have defined

$$\Pi_{ij} \equiv \overline{u_i \frac{\partial p}{\partial x_j}} + \overline{u_j \frac{\partial p}{\partial x_i}}, \qquad C_{ij} = \overline{N_2^i u_j} + \overline{N_2^j u_i}, \qquad \Omega_{ij} \equiv (\epsilon_{ilk}\overline{u_j u_k} + \epsilon_{jlk}\overline{u_i u_k})\Omega_l \tag{A24a}$$

$$\epsilon_\theta \equiv \chi\overline{\left(\frac{\partial \theta}{\partial x_j}\right)^2}, \qquad 2\nu\overline{u_{i,k}u_{j,k}} = \epsilon_{ij}. \tag{A24b}$$

Even though the tensor ϵ_{ij} is usually taken to be diagonal, we prefer to use a slightly more general expression

$$\epsilon_{ij} = \tfrac{2}{3}\epsilon\,\delta_{ij} + (1 - F^{1/2})\epsilon e^{-1} b_{ij}, \tag{A25}$$

where the definition of F is given in Appendix E. The equation for the turbulent kinetic energy $e \equiv \frac{1}{2}\overline{q^2}$, where $q^2 \equiv u_i u_i$, is then

$$\frac{De}{Dt} + \frac{\partial}{\partial x_i}\frac{1}{2}\overline{q^2 u_i} = -\overline{u_i u_j}\frac{\partial U_i}{\partial x_j} + \lambda_i \overline{u_i \theta} - \frac{1}{2}\Pi_{ii} - \epsilon + \frac{1}{2}C_{ii}. \tag{A26}$$

A3. PRESSURE-STRAIN CORRELATIONS

For the tensor Π_{ij} there have been many proposals which have been recently reviewed by Shih & Shabbir (1992), whose formulation we follow:

$$\Pi_{ij} = 2c_4\tau_p^{-1}b_{ij} + (1-\beta_5)B_{ij} - \frac{4}{5}eS_{ij} - \alpha_1\Sigma_{ij} - \alpha_2 Z_{ij}^* + \Pi_{ij}(\mathrm{NL}) + \frac{\partial}{\partial x_j}\overline{pu_i} + \frac{\partial}{\partial x_i}\overline{pu_j}, \tag{A27a}$$

$$\Pi_{ij}(\mathrm{NL}) = -e^{-1}\Pi_{ij}^{\mathrm{nl}} + \lambda_k \Delta_{ij}^k. \tag{A27b}$$

The first term is known as the Rotta (1951) term. The timescale τ_p, which in principle should be determined from the integral of a Green function derived from second-order closure (Herring 1987), is usually taken to be $2e/\epsilon$. However, in the case of stably stratified turbulence, this is no longer true. Weinstock (1978a, b) and Canuto et al. (1993) have suggested that a more physical model requires that

$$\tau_p = \tau(1 + h|N|^2\tau^2)^{-1}, \qquad h = 0.04\delta, \tag{A27c}$$

where $\delta = 0$ for unstable stratification and $\delta = 1$ for stable stratification; N is the Brunt-Vaisala frequency, equation (27c).

The nonlinear contribution Π_{ij}^{nl} and Δ_{ij}^k are given by

$$5\Pi_{ij}^{\mathrm{nl}} = b_{ik}^2 S_{jk} + b_{jk}^2 S_{ik} - 2b_{kj}b_{mi}S_{km} - 3b_{ij}b_{km}S_{km} + b_{ik}^2 R_{jk}^* + b_{jk}^2 R_{ik}^*, \tag{A28}$$

$$\Delta_{ij}^k \equiv -\tfrac{2}{3}(1+4\beta_5)A_{ij}^k + \tfrac{4}{3}(1-\tfrac{1}{2}\beta_5)C_{ij}^k + (\beta_7 + 3\beta_5)D_{ij}^k + \beta_9 E_{ij}^k + e^{-1}(\beta_5 - 1)b_{ij}\overline{\theta u_k} + (\tfrac{3}{2})e^{-2}\beta_5 b_{ij}b_{kp}\overline{\theta u_p}, \tag{A29}$$

where (our b_{ij} is not the same as the b_{ij}^{SL} of Shih & Lumley: $b_{ij} = 2eb_{ij}^{\mathrm{SL}}$)

$$b_{ij} = \overline{u_i u_j} - \tfrac{2}{3}e\,\delta_{ij}, \qquad b_{ij}^2 \equiv b_{ik}b_{jk}, \qquad \tau = 2e/\epsilon, \tag{A30}$$

$$B_{ij} = \lambda_i\overline{u_j\theta} + \lambda_j\overline{u_i\theta} - \tfrac{2}{3}\delta_{ij}\lambda_k\overline{u_k\theta}, \tag{A31}$$

$$\Sigma_{ij} = S_{ik}b_{kj} + S_{jk}b_{ik} - \tfrac{2}{3}\delta_{ij}S_{kl}b_{kl}, \tag{A32}$$

$$Z_{ij}^* = R_{ik}^* b_{kj} + R_{jk}^* b_{ik} - \tfrac{2}{3}\delta_{ij}R_{kl}^* b_{kl}, \tag{A33}$$

$$2S_{ij} = U_{i,j} + U_{j,i}, \qquad R_{ij}^* = \omega_{ij} - \epsilon_{ijk}\Omega_k, \qquad 2\omega_{ij} = U_{i,j} - U_{j,i}, \tag{A34}$$

$$2eA_{ij}^k \equiv b_{ik}\overline{\theta u_j} + b_{jk}\overline{\theta u_i} - \tfrac{2}{3}\delta_{ij}b_{pk}\overline{\theta u_p}, \tag{A35}$$

$$2eC_{ij}^k \equiv (\delta_{ik}b_{jp} + \delta_{jk}b_{ip} - \tfrac{2}{3}\delta_{ij}b_{kp})\overline{u_p\theta}, \tag{A36}$$

$$4e^2 D_{ij}^k \equiv [b_{ik}b_{jp} + b_{jk}b_{ip} - (\delta_{ik}b_{jm} + \delta_{jk}b_{im})b_{mp}]\overline{u_p\theta}, \tag{A37}$$

$$4e^2 E_{ij}^k \equiv (b_{im}\overline{u_j\theta} + b_{jm}\overline{u_i\theta})b_{mk} - (\delta_{ik}b_{jm} + \delta_{jk}b_{im})b_{mp}\overline{u_p\theta}, \tag{A38}$$

$$\Delta_{ii}^k = 0. \tag{A39}$$

Putting together equations (23), (26), and (27), we obtain the dynamic equation for the tensor b_{ij}

$$\frac{D}{Dt}b_{ij} + D_f(b_{ij}) = -2c_4^*\tau_p^{-1}b_{ij} + \beta_5 B_{ij} - \frac{8}{15}eS_{ij} - (1-\alpha_1)\Sigma_{ij} - (1-\alpha_2)Z_{ij} - \Pi_{ij}(\mathrm{NL}) + C_{ij} - \frac{1}{3}\delta_{ij}C_{kk}, \tag{A40a}$$

where

$$D_f(b_{ij}) \equiv \frac{\partial}{\partial x_k}\left[\left(\overline{u_i u_j u_k} - \frac{1}{3}\delta_{ij}\overline{q^2 u_k}\right) + \left(\delta_{ik}\overline{pu_j} + \delta_{jk}\overline{pu_i} - \frac{2}{3}\delta_{ij}\overline{pu_k}\right)\right], \tag{A40b}$$

$$Z_{ij} \equiv b_{ik}\omega_{jk} + b_{jk}\omega_{ik} - (2-\alpha_2)(1-\alpha_2)^{-1}(\epsilon_{jkl}b_{ik} + \epsilon_{ikl}b_{jk})\Omega_l. \tag{A40c}$$

The constants are discussed in Appendix E. Analogously,

$$\Pi_i^\theta \equiv \overline{\theta \frac{\partial p}{\partial x_i}} = f_1 \tau_p^{-1} \overline{u_i \theta} + \gamma_1 \lambda_i \overline{\theta^2} - \frac{3}{4} \alpha_3 \left(S_{ik} + \frac{5}{3} R_{ik}^* \right) \overline{u_k \theta} + \Pi_i^\theta(\mathrm{NL}) + \frac{\partial}{\partial x_i} \overline{p\theta} - (\nu + \chi) \overline{\frac{\partial \theta}{\partial x_k} \frac{\partial u_i}{\partial x_k}} , \tag{A41}$$

where

$$\Pi_i^\theta(\mathrm{NL}) \equiv \lambda_j Y_{ij} + e^{-1}(S_{jk} + R_{jk}^*)(\alpha_4 B_{ij}^k - \alpha_6 b_{ij} \overline{\theta u_k}) , \tag{A42a}$$

$$4e Y_{ij} \equiv 2\gamma_2 \overline{\theta^2} b_{ij} + 4\gamma_3 \overline{\theta u_i}\, \overline{\theta u_j} + 2\gamma_4 e^{-1}(b_{ik} \overline{\theta u_j}\, \overline{\theta u_k} + b_{jk} \overline{\theta u_i}\, \overline{\theta u_k}) + \gamma_5 e^{-1} b_{ik} b_{kj} \overline{\theta^2} , \tag{A42b}$$

$$B_{ij}^k \equiv b_{ik} \overline{\theta u_j} + b_{jk} \overline{\theta u_i} - \tfrac{2}{3} \delta_{ij} b_{kp} \overline{\theta u_p} . \tag{A42c}$$

If we neglect the nonlinear terms by taking

$$\gamma_2 = \gamma_3 = \gamma_4 = \gamma_5 = 0 , \tag{A43}$$

we recover equations (43a) (Paper I), if we further call $f_1 \equiv 2c_6$ and $\gamma_1 \equiv c_7$. Inserting equation (A41) into equation (A16) above, we finally obtain the equation for $\overline{u_i \theta}$, namely,

$$\frac{D}{Dt} \overline{u_i \theta} + D_f(\overline{u_i \theta}) = -\left(\overline{u_i u_j} \frac{\partial T}{\partial x_j} + \overline{u_j \theta} \frac{\partial U_i}{\partial x_j} \right) - f_1 \tau_p^{-1} \overline{u_i \theta} + (1 - \gamma_1) \lambda_i \overline{\theta^2}$$
$$+ \frac{3}{4} \alpha_3 \left(S_{ij} + \frac{5}{3} R_{ij}^* \right) \overline{u_j \theta} - 2\epsilon_{ijk} \overline{u_k \theta} \Omega_j - \Pi_i^\theta(\mathrm{NL}) + \frac{1}{2} (\nu + \chi) \frac{\partial^2}{\partial x_j^2} \overline{u_i \theta} + C_i , \tag{A45a}$$

$$D_f(\overline{u_i \theta}) = \frac{\partial}{\partial x_j} (\overline{\theta u_i u_j} + \delta_{ij} \overline{p\theta}) . \tag{A45b}$$

APPENDIX B

THE C TERMS

First, let us consider C^θ. Using the definition, equation (A21), and Paper I equation (38b), we derive (for ease of notation, we take $\rho = 1$)

$$\frac{1}{2} c_p C^\theta = (\overline{u_j \theta} + \alpha \overline{u_j \theta^2}) \frac{\partial P}{\partial x_j} + \frac{1}{2} \Pi_{ii}^\theta + \overline{\epsilon \theta} . \tag{B1}$$

With the aid of equation (44f) (Paper I):

$$\tfrac{1}{2} \Pi_{ii}^\theta = -3c_9 \tau^{-1} \overline{q^2 \theta} , \tag{B2}$$

and of the closure $\overline{\epsilon \theta} = \tau^{-1} \overline{q^2 \theta}$, we finally obtain

$$\frac{1}{2} c_p C^\theta = (\overline{u_j \theta} + \alpha \overline{u_j \theta^2}) \frac{\partial P}{\partial x_j} + (1 - 3c_9) \tau^{-1} \overline{q^2 \theta} , \tag{B3}$$

where the pressure gradient must be obtained from equation (A6).

We shall write equation (B3) as

$$\frac{1}{2} c_p C^\theta = \overline{u_j \theta} \frac{\partial P}{\partial x_j} + \text{third-order moments} . \tag{B4}$$

From equation (A6) in the stationary case and to the lowest order, we derive

$$\frac{\partial P}{\partial x_i} = -g_i - 2\epsilon_{ijk} \Omega_j U_k , \tag{B5}$$

so that to the lowest order

$$\tfrac{1}{2} C^\theta = -c_p^{-1} \overline{u_i \theta} (g_i + 2\epsilon_{ijk} \Omega_j U_k) . \tag{B6}$$

The first term serves to renormalize the first term on the right-hand side of equation (21) via the introduction of the adiabatic temperature gradient, a fact that we have used in going from equation (35) to equation (36a).

Next, consider C_{ii}, defined in equation (A24). Using Paper I, equations (38b) and (44f), one obtains

$$\frac{1}{2} C_{ii} = -\alpha g_i \overline{\theta u_i} + \left(\frac{1}{P} \overline{p u_i} - \alpha \overline{\theta u_i} \right) \frac{\partial P}{\partial x_i} + 3c_9 \tau^{-1} \alpha \overline{q^2 \theta} , \tag{B7}$$

where

$$\overline{pu_i} = -C_p^w \overline{q^2 u_i} , \tag{B8}$$

with the gradient of the pressure given by equation (A6) or, approximately, by equation (B5) above. To the lowest order, only rotation contributes to C_{ii}.

Finally, let us consider C_i (eq. [A18]). Using Paper I, equations (39b) and (45), we derive

$$C_i = c_p^{-1}\overline{u_i u_j}\frac{\partial P}{\partial x_j} - \alpha\overline{\theta^2}\left(g_i + \frac{\partial P}{\partial x_i}\right) + \text{third-order terms} , \tag{B9}$$

where

$$\text{third-order terms} = \left(\frac{1}{P}\overline{p\theta} + c_p^{-1}\alpha\overline{\theta u_i u_j}\right)\frac{\partial P}{\partial x_j} - 2c_8\alpha\tau^{-1}\overline{u_i\theta^2} - c_{11}\alpha\lambda_i\overline{\theta^3} + c_p^{-1}\left(\tau^{-1}\overline{u_i q^2} + \overline{u_i u_j \frac{\partial p}{\partial x_j}}\right), \tag{B10}$$

where the last term in equation (B10) must be computed using Paper I, equations (37b) and (44e). To the lowest order given by equation (B5) above, equation (B9) becomes

$$C_i = -c_p^{-1} g_j \overline{u_i u_j} , \tag{B11}$$

which serves to renormalize the first term in equation (32) by introducing the adiabatic temperature gradient, equation (36c).

APPENDIX C

THE DISSIPATION RATES ϵ AND ϵ_θ

C1. UNSTABLE STRATIFICATION

An equation for ϵ was first proposed by Davidov (1961). With the addition of buoyancy, its more popular form reads (Zeman & Lumley 1976; Lumley 1978; Launder 1990; Speziale, Gatski, & Sarkar 1992)

$$\frac{D}{Dt}\epsilon + \frac{\partial}{\partial x_j}(\overline{\epsilon u_j}) = C_{\epsilon_1}\frac{\epsilon}{e}P - C_{\epsilon_2}\frac{\epsilon^2}{e} . \tag{C1}$$

P means total production,

$$P = P_b + P_s , \tag{C2}$$

where the buoyancy and shear contributions are defined as

$$\text{buoyancy: } P_b = \lambda_i\overline{\theta u_i} , \tag{C3}$$

$$\text{shear: } P_s = -b_{ij}S_{ij} . \tag{C4}$$

The ratio

$$R_f = -\frac{P_b}{P_s} = \frac{\lambda_i\overline{u_i\theta}}{b_{ij}S_{ij}} \tag{C5}$$

is the flux Richardson number.

If one adopts a down-gradient–like approximation, namely,

$$\overline{\epsilon w} = -\kappa_t\frac{\partial\epsilon}{\partial z} , \tag{C6}$$

where κ_t is a turbulent diffusivity, equation (C1) takes its standard form. Since κ_t has dimensions of wl, dimensional analysis applied to equation (C1) yields

$$\epsilon \sim e^{3/2}l^{-1} . \tag{C7}$$

Introducing the timescale (A30)

$$\tau = 2e/\epsilon , \tag{C8}$$

equation (C1) can be transformed into an equation for τ:

$$\frac{D\tau}{Dt} + \tau(e^{-1}D_f e - \epsilon^{-1}D_f\epsilon) = 2(C_{\epsilon_2} - 1) - 2(C_{\epsilon_1} - 1)\frac{P}{\epsilon} + \frac{1}{\epsilon}C_{ii} , \tag{C9}$$

where D_f means diffusion, i.e.,

$$D_f \epsilon \equiv \frac{\partial}{\partial x_i} (\overline{\epsilon u_i}) , \qquad D_f e \equiv \frac{\partial}{\partial x_i} (\overline{e u_i} + \overline{p u_i}) . \tag{C10}$$

The equation for ϵ_θ is given by (Zeman & Lumley 1979)

$$\frac{D}{Dt} \epsilon_\theta + \frac{\partial}{\partial x_j} (\overline{\epsilon_\theta u_j}) = -b_1 \epsilon_\theta \tau_\theta^{-1}\left(1 + \frac{1}{4}\frac{\tau_\theta}{\tau}\right) + b_2(\epsilon\tau^3)^{-1}(\overline{w\theta})^2 - b_3 \tau_\theta^{-1}\overline{w\theta}\,\frac{\partial T}{\partial z} + \chi\nabla^2\epsilon_\theta , \tag{C11}$$

where the relations analogous to equations (C5) and (C6) are

$$\overline{\epsilon_\theta w} = -K_h \frac{\partial}{\partial z} \epsilon_\theta , \tag{C12}$$

$$K_h = -\overline{\theta^2 w}\bigg/\left(\frac{\partial \overline{\theta^2}}{\partial z}\right) . \tag{C13}$$

It must be noted that some authors (e.g., Andre, Lacarrere, & Traore 1982) use much simpler relations, namely,

$$\epsilon = \frac{e^{3/2}}{l_\epsilon} , \qquad \epsilon_\theta = \frac{1}{2} c_\theta \overline{\theta^2} \frac{e^{1/2}}{l_\epsilon} = \frac{1}{2} c_\theta \overline{\theta^2} \epsilon e^{-1} . \tag{C14}$$

In the LES + SGS approach, one usually identifies

$$l_\epsilon = c_\epsilon^{-1}\Delta , \tag{C15}$$

where Δ is the smallest resolved scale. The constant c_ϵ is determined by considering that the subgrid kinetic energy is defined as

$$e = \int_{\pi/\Delta}^{\infty} E(k)dk . \tag{C16}$$

If one assumes that the subgrid scales are inertial (Ko is the Kolmogorov constant),

$$E(k) = \mathrm{Ko}\,\epsilon^{2/3}k^{-5/3} , \tag{C17}$$

substitution of equation (C17) into equation (C16) yields equation (C13) with

$$c_\epsilon = \pi\left(\frac{2}{3\,\mathrm{Ko}}\right)^{3/2} . \tag{C18}$$

Analogously, we have for the temperature field

$$\overline{\theta^2} = \int_{\pi/\Delta}^{\infty} G(k)dk , \tag{C19}$$

$$G(k) = \mathrm{Ba}\ \epsilon_\theta \epsilon^{-1/3} k^{-5/3} , \tag{C20}$$

so that we recover the second equation of (C14) with

$$\frac{1}{2} c_\theta = c_\epsilon \frac{\mathrm{Ko}}{\mathrm{Ba}} , \tag{C21}$$

where Ba is the Batchelor constant (Monin & Yaglom 1971, 1975).

Expression (C13) with equations (15), (18), and (21) have been successfully applied in LES calculations. However, these relations cease to be correct in the presence of stable stratification.

C2. STABLE STRATIFICATION, GRAVITY WAVES

Stably stratified turbulence, like that encountered in the overshooting regions in stellar interiors, cannot be described by equation (C13) because a new phenomenon comes into play, *negative buoyancy*, which forces the eddies to work against gravity and lose kinetic energy which goes to feed density fluctuations (*gravity waves*). This means that the basic ingredients (eqs. [C17] and [C20]) are no longer valid since the SGS eddies are no longer inertial.

The first to present a model to account for the effects of stable stratification were Bolgiano (1959, 1962), Shur (1962), and Lumley (1964). Since there are difficulties with Bolgiano's model (for a review, see Phillips 1965), one usually considers Lumley's theory, which however predicts a unique k^{-3} power law for the buoyancy subrange. While atmospheric and oceanographic data (Gargett et al. 1981; Gargett 1985, 1989, 1990; Weinstock 1978a, b; 1985a, b; Dalaudier & Sidi 1987) are in qualitative agreement with this prediction, they actually exhibit spectral indices ranging from -2.5 to -3. Lumley's theory was critically analyzed by Weinstock (1978a, b, 1980, 1985a, b, 1990) who pointed out, among other things, that a physically complete treatment of a stably stratified flow must explicitly account for the gravity waves that ultimately store the kinetic energy lost by the eddies.

A further complication comes from the fact that, while negative buoyancy (a sink) always makes the eddies lose a fraction of their energy, shear (a source) acts to restore it, and thus, depending on the value of the Richardson number R_f, the model may behave differently. At present, there are three models.

Small-to-moderate buoyancy.—$R_f \le \frac{1}{3}$. Deardorff (1980) suggested that in this case one can still use the Smagorinsky model (eq. [59]) provided the length scale l is taken to be

$$l = \min(\Delta, l_b)\,, \qquad l_b = 0.76\,\frac{e^{1/2}}{N}\,, \tag{C22}$$

which implies that stable stratification *decreases the master length.*

Strong buoyancy, no shear.—$R_f = \infty$. In this case, Canuto & Minotti (1993) have derived the following expression for l_ϵ

$$l = \Delta \exp(bx^2)\,, \tag{C23a}$$

$$x = (-N^2)^{1/2}\Delta e^{-1/2}\,, \qquad b \equiv \frac{9}{35\pi^2}\,\mathrm{Ko}^{3/2}\,, \tag{C23b}$$

which implies that stable stratification *increases the master length* (with respect to Δ).

Arbitrary values of R_f.—Recently, Cheng & Canuto (1993) have derived a general expression for l. The result is

$$l_\epsilon = c_\epsilon^{-1} l\,, \qquad l/\Delta = \Gamma(\mathrm{Fr}, R_f)\,, \qquad c_\epsilon = \mathrm{const.}\,, \tag{C24a}$$

where

$$\mathrm{Fr} = \frac{e^{1/2}}{\Delta N}\,, \qquad R_f = \frac{\lambda_i \overline{u_i\theta}}{b_{ij}S_{ij}}\,, \qquad N^2 = -\alpha g_i\left[\frac{\partial T}{\partial x_i} - \left(\frac{\partial T}{\partial x_i}\right)_{\mathrm{ad}}\right]. \tag{C24b}$$

Fr is the Froude number, R_f is the flux Richardson number, and N is the Brunt-Vaisala frequency ($N^2 > 0$ for unstable stratification and $N^2 < 0$ for stable stratification); $\lambda_i = g_i\alpha$, $g_i = (0, 0, g)$, and α is the volume expansion coefficient. Δ can be considered *the limit of l in the neutral and shearless case.*

The function Γ is given by (Cheng & Canuto 1993)

$R_f < R_{fc}$:

$$\Gamma \equiv [1 + a\,\mathrm{Fr}^{-2}(1 + b\,\mathrm{Fr}^{-4/3})^{-1}]^{-3/2}\,, \qquad 3\pi^2 a = 2(A-1)\,, \qquad b = 0.12\,|A - 1 + \tfrac{3}{2}A^{-1}|^{4/9} \tag{C25}$$

$R_f > R_{fc}$:

$$\Gamma \equiv [1 + (4/5\pi^2)A\,\mathrm{Fr}^{-2}]^c\,, \qquad c = \tfrac{5}{4}(A^{-1} - 1)\,. \tag{C26}$$

In both expressions A is defined as

$$A \equiv 1 + (3^{1/2}/4)\,\mathrm{Ko}^{3/2}\,[(R_{fc}/R_f) - 1]\,. \tag{C27}$$

Cheng & Canuto (1993) have also shown how the expression for l does reproduce the empirical expressions suggested by Deardorff (1980) and Hunt et al. (1988).

APPENDIX D

THIRD-ORDER MOMENTS

The equations for the third-order moments are taken from Paper I. We have

$$\left(\frac{D}{Dt} + \tau_3^{-1}\right)\overline{u_iu_ju_k} = -(\overline{u_iu_ju_l}\,U_{k,l} + \mathrm{perm.}) - \left(\overline{u_iu_l}\,\frac{\partial}{\partial x_l}\,\overline{u_ju_k} + \mathrm{perm.}\right) + (1 - c_{11})(\lambda_i\overline{\theta u_ju_k} + \mathrm{perm.}) - 2\Omega_{ijk} - \frac{2}{3\tau}(\delta_{ij}\overline{q^2u_k} + \mathrm{perm.})\,, \tag{D1}$$

$$\left(\frac{D}{Dt} + \tau_3^{-1}\right)\overline{u_iu_j\theta} = \overline{u_iu_ju_k}\,\beta_k - (\overline{u_iu_k\theta}\,U_{j,k} + \overline{u_ju_k\theta}\,U_{i,k}) - \left(\overline{u_iu_k}\,\frac{\partial}{\partial x_k}\,\overline{\theta u_j} + \overline{u_ju_k}\,\frac{\partial}{\partial x_k}\,\overline{\theta u_i} + \overline{\theta u_k}\,\frac{\partial}{\partial x_k}\,\overline{u_iu_j}\right)$$
$$+ \frac{2}{3}\,c_{11}\,\delta_{ij}\lambda_k\overline{\theta^2u_k} + \tau^{-1}c_*\,\delta_{ij}\overline{q^2\theta} + (1 - c_{11})(\lambda_i\overline{\theta^2u_j} + \lambda_j\overline{\theta^2u_i}) - 2\Lambda_{ij}\,, \tag{D2}$$

$$\left(\frac{D}{Dt} + \tau_3^{-1} + 2\tau_\theta^{-1}\right)\overline{u_i\theta^2} = 2\overline{\theta u_iu_j}\,\beta_j - \overline{\theta^2u_j}\,U_{i,j} - 2\overline{\theta u_j}\,\frac{\partial}{\partial x_j}\,\overline{\theta u_i} + (1 - c_{11})\lambda_i\overline{\theta^3} - \overline{u_iu_j}\,\frac{\partial}{\partial x_j}\,\overline{\theta^2} - 2\epsilon_{ijk}\Omega_j\overline{u_k\theta^2}\,, \tag{D3}$$

$$\left(\frac{D}{Dt} + \frac{c_{10}}{c_8}\,\tau_3^{-1}\right)\overline{\theta^3} = 3\overline{\theta^2u_j}\,\beta_j - 3\overline{\theta u_j}\,\frac{\partial}{\partial x_j}\,\overline{\theta^2} + \chi\,\frac{\partial^2}{\partial x_l^2}\,\overline{\theta^3}\,, \tag{D4}$$

where β_i has been defined in the text, equation (36c), and

$$U_{i,j} \equiv \frac{\partial U_i}{\partial x_j}\,, \qquad \tau = \frac{2e}{\epsilon}\,, \qquad \tau_3 \equiv \frac{\tau}{2c_8}\,, \qquad \tau_\theta = \frac{\overline{\theta^2}}{\epsilon_\theta}\,,$$

$$\Lambda_{ij} = (\epsilon_{ilk}\overline{u_j u_k \theta} + \epsilon_{jlk}\overline{u_i u_k \theta})\Omega_l\,, \qquad \Omega_{ijk} = (\epsilon_{ilm}\overline{u_j u_k u_m} + \text{perm.})\Omega_l\,, \qquad c_* = (2/3)(c_8 + 3c_9 - c_{10})\,. \tag{D5}$$

In the stationary case, it has been customary for many years to approximate equations (D1)–(D3) with

$$\overline{u_i u_j u_k} \to -\tau_3 \overline{u_k u_l}\frac{\partial}{\partial x_l}\overline{u_i u_j}\,, \qquad \overline{u_i u_j \theta} \to -\tau_3 \overline{u_j u_k}\frac{\partial}{\partial x_k}\overline{\theta u_i}\,, \qquad \overline{u_i \theta^2} \to -\tau_3(1 + 2\tau_3\tau_\theta^{-1})\overline{u_i u_j}\frac{\partial}{\partial x_j}\overline{\theta^2}\,. \tag{D6}$$

If the degree of anisotropy is assumed to be small,

$$b_{ij} = \overline{u_i u_j} - \tfrac{2}{3}e\,\delta_{ij} \approx 0\,, \tag{D7}$$

one further has

$$\overline{u_i u_j u_k} \to -A\nu_t \frac{\partial}{\partial x_k}\overline{u_i u_j}\,, \qquad \overline{u_i u_j \theta} \to -A\nu_t \frac{\partial}{\partial x_j}\overline{\theta u_i}\,, \qquad \overline{u_i \theta^2} \to -B\nu_t \frac{\partial}{\partial x_i}\overline{\theta^2}\,, \tag{D8}$$

with $3c_8 c_\nu A \equiv 2$ and $B \equiv A(1 + 2\tau_3\tau_\theta^{-1})$; the turbulent viscosity ν_t is given by equation (44a) with $\Sigma_b = 0$. Equations (D6) and (D8) represent the *down-gradient, diffusive approximation to the third-order moments.*

As discussed in Paper I, equations (D8) lead to incorrect results: for example, planetary boundary layer data show that

$$\overline{w^3} > 0 \qquad \text{and} \qquad \frac{\partial}{\partial z}\overline{w^2} > 0\,, \tag{D9}$$

which contradict the first of equation (D8). Recently, the system (D1)–(D4) has been inverted exactly in the case in which there is no mean flow and the variables depend only on z (Canuto et al. 1993). The principal result is that all third-order moments exhibit a universal structure: they all are a linear combination of the gradients of all the second-order moments. For example,

$$\overline{q^2 w} = D_1 \frac{\partial}{\partial z}\overline{w^2} + D_2 \frac{\partial}{\partial z}\overline{q^2} + D_3 \frac{\partial}{\partial z}\overline{w\theta} + D_4 \frac{\partial}{\partial z}\overline{\theta^2}\,, \tag{D10}$$

where the turbulent diffusivities D_k have the general structure

$$D \approx a\nu_t + b\overline{w\theta}\,, \tag{D11}$$

indicating that the turbulent diffusivities are contributed not only by the mechanical part $\nu_t \sim wl$, but also by buoyancy.

The approximations

$$U_i = 0\,, \qquad \frac{\partial}{\partial x_i} \to \frac{\partial}{\partial z}\,, \tag{D12}$$

can be made in an ensemble-average approach, but not in the context of an LES where all the components of U_i and *all* the space dependence must be kept. Infact U_i does not represent an external field but the large scales. This makes the inversion of equations (D1)–(D4) a harder task, even with the help of symbolic algebra. Until that is done, we suggest the use of a temporary intermediate solution between equation (D6) and (D10). The idea is to begin with the down-gradient approximation as a zero-order solution ($n = 0$) to be substituted back into all the third-order moments appearing on the right-hand sides of equations (D1)–(D4). This will provide, without the need of a matrix inversion, a new set of third-order moments

$$\overline{u_i u_j u_k}\,, \qquad \overline{u_i u_j \theta}\,, \qquad \overline{u_i \theta^2}\,. \tag{D13}$$

The calculation cannot, however, be stopped at this stage. In fact, one can notice that at this level of approximation, one would not recover all the terms appearing in equation (D10): for example, the first third-order moment in equation (D13) would not contain the last term in equation (D10), namely, the gradient of the temperature variance, as one observes by inspecting the components of the zero-order expression for $\overline{u_i u_j \theta}$. On the other hand, if one goes a step further, such a dependence is recovered.

Formally, the procedure can be written as follows: define

$$A_{ijk} \equiv \overline{u_i u_j u_k}\,, \qquad B_{ij} \equiv \overline{\theta u_i u_j}\,, \qquad C_i \equiv \overline{u_i \theta^2}\,, \qquad D \equiv \overline{\theta^3}\,. \tag{D14}$$

Then we have from equation (D1)

$$A_{ijk}^{n+1} = A_{ijk}^0 - \tau_3(A_{ijl}^n U_{k,l} + \text{perm.}) + (1 - c_{11})\tau_3(\lambda_i B_{jk}^n + \text{perm.}) - 2(\epsilon_{ilm} A_{jkm}^n + \text{perm.})\tau_3\Omega_l - (1/3c_8)(\delta_{ij} A_{ppk}^n + \text{perm.})\,, \tag{D15}$$

where the zeroth-order approximations (which include the down-gradient as a subcase) are defined as

$$-\tau_3^{-1} A_{ijk}^0 \equiv \overline{u_i u_l}\frac{\partial}{\partial x_l}\overline{u_j u_k} + \text{perm.}\,, \tag{D16}$$

$$-\tau_3^{-1}B_{ij}^0 \equiv \overline{u_i u_k}\frac{\partial}{\partial x_k}\overline{\theta u_j} + \overline{u_j u_k}\frac{\partial}{\partial x_k}\overline{\theta u_i} + \overline{\theta u_k}\frac{\partial}{\partial x_k}\overline{u_i u_j}, \tag{D17}$$

$$-\tau_3^{-1}(1 + 2\tau_3\tau_\theta^{-1})C_i^0 \equiv 2\overline{\theta u_j}\frac{\partial}{\partial x_j}\overline{\theta u_i} + \overline{u_i u_j}\frac{\partial}{\partial x_j}\overline{\theta^2}, \tag{D18}$$

$$-\frac{c_{10}}{c_8}\tau_3^{-1}D^0 \equiv 3\overline{\theta u_j}\frac{\partial}{\partial x_j}\overline{\theta^2}. \tag{D19}$$

Analogously equation (D2) becomes, with $c_* = 0$,

$$B_{ij}^{n+1} = B_{ij}^0 + \beta_k\tau_3 A_{ijk}^n - \tau_3(B_{ik}^n U_{j,k} + B_{jk}^n U_{i,k}) + \tfrac{2}{3}c_{11}\delta_{ij}\tau_3\lambda_k C_k^n + (1 - c_{11})\tau_3(\lambda_i C_j^n + \lambda_j C_i^n) - 2(\epsilon_{ilk}B_{jk}^n + \epsilon_{jlk}B_{ik}^n)\tau_3\Omega_l. \tag{D20}$$

Equation (D3) becomes

$$C_i^{n+1} = C_i^0 + T[2\beta_j B_{ij}^n - C_j^n U_{i,j} + (1 - c_{11})\lambda_i D^n - 2\epsilon_{ijk}\Omega_j C_k^n], \tag{D21}$$

where

$$T \equiv \tau_3(1 + 2\tau_3/\tau_\theta)^{-1}. \tag{D22}$$

Finally, equation (D4) becomes

$$D^{n+1} = D^0 + (3c_8/c_{10})\tau_3\beta_i C_i^n. \tag{D23}$$

The remaining third-order moments are determined by the relations

$$\overline{pu_i} = -C_p^w\overline{q^2u_i}, \qquad \overline{p\theta} = -C_p^\theta\overline{q^2\theta}. \tag{D24}$$

APPENDIX E

1. Equations (23)–(26):

$$c_4^* = c_4 + (1 - F^{1/2})\tau_p\tau^{-1}, \qquad c_4 = 1 + 6.22F^2(1 - F)^{3/4}, \qquad f_1 = 7.5,$$
$$\alpha_1 = 6\alpha_5, \quad 3\alpha_2 = 2(2 - 7\alpha_5), \quad \alpha_3 = \tfrac{4}{5}, \quad \alpha_4 = \tfrac{3}{10}, \quad 10\alpha_5 = 1 + \tfrac{4}{5}F^{1/2}, \quad \alpha_6 = \tfrac{1}{10},$$
$$F = 1 + 9\mathrm{II} + 27\mathrm{III}. \tag{E1}$$

The invariants II and III are defined below (eq [E8]). For two-dimensional turbulence $F \sim 0$.

2. Equations (23)–(26): constants entering the third-order moments (Eq. A46] and Appendix D)

$$c_8 = 8, \qquad c_{10} = 4, \qquad c_{11} = \tfrac{1}{5}, \qquad c_* = 0, \qquad C_p^w = C_p^\theta = \tfrac{1}{5}. \tag{E2}$$

3. Equations (23)–(26): the functions γ entering equations (26) and the nonlinear term Y_i^{nl}, equation (42) (Shih & Shabbir 1992):

$$9\gamma_1 \equiv 6r^2 - 10 - \beta_5(r^2 - 1)^{-1}[18(r^2 + 1)rb + r^2(7 - 15r^2) + 36\mathrm{II} - 10], \tag{E3}$$

$$9(r^2 - 1)\mathrm{II}\gamma_2 \equiv r^2(3\mathrm{II} + 14) - (3\mathrm{II} + \tfrac{7}{2}) - \tfrac{21}{2}r^4 - \beta_5[r^2(12\mathrm{II} + 20) + 108\mathrm{II}rb + 108\mathrm{II}^2 - 21\mathrm{II} - 5 - 15r^4(1 + 3\mathrm{II})], \tag{E4}$$

$$\gamma_3 \equiv -1 + \tfrac{1}{2}\beta_5(r^2 - 1)^{-1}(12rb - 5r^2 + 12\mathrm{II} - 1), \tag{E5}$$

$$\gamma_4 \equiv -\tfrac{3}{2}\beta_5, \qquad 6\mathrm{II}\gamma_5 \equiv 7 + \beta_5(36\mathrm{II} - 10), \tag{E6}$$

where

$$2r^2 \equiv \overline{\theta u_i}\,\overline{\theta u_i}(\overline{\theta^2}e)^{-1}, \qquad 2rb \equiv (\overline{\theta^2}e)^{-1}\overline{\theta u_i}\,\overline{\theta u_j}b_{ij}, \tag{E7}$$

$$-8e^2\mathrm{II} \equiv b_{ij}b_{ij}, \qquad 24e^3\mathrm{III} \equiv b_{ij}b_{jk}b_{ki}. \tag{E8}$$

Using data from a buoyant plume experiment, Shih & Shabbir (1992) have determined that the value of β_5 is approximately 0.6, which would correspond to $c_5 \equiv 1 - \beta_5 = 0.4$, a value close to 0.3 suggested in Paper I, equation (44d). In the same work, the authors have also shown that γ_1 is almost constant ($\sim$0.42), while $\gamma_2, \gamma_3, \gamma_4$, and γ_5 are all negative, with values ranging as follows:

$$1.91 < |\gamma_2| < 2.82, \qquad 0.28 < |\gamma_3| < 0.7, \qquad 0.81 < |\gamma_4| < 2.76, \qquad 0.95 < |\gamma_5| < 3.15. \tag{E9}$$

4. Equations (23)–(26): the functions β_5, β_7, and β_9 entering equation (25) and the nonlinear term Δ_{ij}^k (eq. [A29]) (Shih & Shabbir 1992), are given by

$$\beta_5(6\mathrm{II} - 10r^2 - 36\mathrm{II}rb) = -(12\mathrm{II} + 7)r^2, \tag{E10}$$

$$\mathrm{II}\beta_7 = -\tfrac{7}{6} + \beta_5(\tfrac{5}{3} - \mathrm{II}), \tag{E11}$$

$$-\beta_9 = \beta_5 + \beta_7 \, . \tag{E12}$$

5. Equations (27a) and (27b):

$$c_\epsilon = \pi\left(\frac{2}{3\,\mathrm{Ko}}\right)^{3/2} , \quad \frac{1}{2}\, c_\theta = c_\epsilon \frac{\mathrm{Ko}}{\mathrm{Ba}} , \quad \mathrm{Ko} = 1.6 \pm 0.02 \, , \quad \mathrm{Ba} = 1.34 \pm 0.02 \, . \tag{E13}$$

The values of Ko and Ba are taken from Andreas (1987).

6. Appendix C: the constants

$$C_{\epsilon_1} = 1.44 \, , \quad C_{\epsilon_2} = 1.83 \, , \tag{E14}$$

$$b_1 = 3 \, , \quad b_2 = 30 \, , \quad b_3 = 0.97 \, . \tag{E15}$$

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